

Development of an  
ENVIRONMENT-ACCIDENT INDEX

A planning tool to protect the environment  
in case of a chemical accident

by

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Akademisk avhandling

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**Title** Development of an Environment-Accident Index - A planning tool to protect the environment in case of a chemical accident.

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### **Abstract**

The increasing mass and complexity of chemicals being produced and transported has resulted in more rigorous demands on both authorities as well as chemical-handling industries to assess the risks involved. The Environment-Accident Index (EAI), has been proposed as a planning tool created as an equation in which chemical properties (variables describing the chemical involved) are combined with site-specific properties (variables describing the accident site). The EAI is intended to facilitate assessment of the environmental effects related to chemical accident scenarios and hence assist the organisation of preventative programs. The main objective of the work described in this thesis was to evaluate, develop and improve the proposed EAI. The steps involved in the development process included I) evaluation of the feasibility of the EAI approach, II) selection of a representative and diverse set of chemical accidents to be used in the development III) the use of questionnaires and expert judgements to develop response values for environmental effects of a chemical accident, and IV) to create a new EAI model using multivariate modelling (PLS). The EAI approach proved to be useful in the work to protect the environment in case of a chemical accident. A representative set of accidents was selected by means of statistical multivariate design (PCA) based on assembled data related to a set of 55 chemical accidents. The selection generated a set of accidents representing a diverse spectrum of chemical accident scenarios. To develop a measure of environmental effects of the chemical accidents i.e. responses, an expert panel was asked to judge their environmental effects (such as effects on animal life in the aquatic or terrestrial environment). The results showed that the judgements give a rough estimate of environmental effects that could be used as responses in the development of the EAI. The developed responses were then related to the chemical and site-specific properties to create a new EAI model. This resulted in a PLS-based EAI connected to a new classification scale. The advantages of the new EAI are that it can be calculated without the use of tables; it can estimate the effects for all included responses, and make a rough classification of chemical accidents according to the new classification scale. Finally, the new EAI is a more stable model than the previously proposed EAI, and it is founded on a valid base of accident scenarios, making its use for a variety of chemicals and situations more reliable since it covers a broader spectrum of accident scenarios. The new EAI can be expressed as a regression model to facilitate calculation of the index for people that do not have access to PLS. The highest priorities for further refining the new EAI in the future are: external validation of the EAI; further refinement of the formula's structure; adjustment of the new classification scale; and real-life evaluation of the EAI.

**Keywords** Environment-Accident Index, chemical accidents, environmental effects, questionnaire, expert judgements, statistical multivariate design, PCA, PLS

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**Titel** Utveckling av Miljöolycksindex - ett planeringsverktyg för att skydda miljön i händelse av kemikalieolycka.

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### **Sammanfattning**

Ett ständigt ökande kemikalieflöde har resulterat i allt hårdare krav på både myndigheter och kemikalieindustrin att kunna bedöma de risker som kemikaliehantering medför. Miljöolycksindex (MI) är ett planeringsverktyg som baseras på att kemikalieegenskaper och områdesspecifika egenskaper vägs samman i en enkel formel. MI kan användas som hjälp för att bedöma miljöeffekter relaterade till en kemikalieolycka och därmed underlätta det förebyggande arbetet för myndigheter och industri. Syftet med denna avhandling var att utveckla och förbättra MI. De olika stegen i detta arbete inkluderar I) utvärdering av möjligheten att använda MI II) val av ett representativt set av kemikalieolyckor att användas i utvecklingen av MI III) använda frågeformulär kombinerat med en expertpanel för att ta fram ett mått på miljöeffekter kopplat till kemikalieolyckor (sk responser) och IV) att skapa en ny MI modell med hjälp av multivariat modellering (PLS). Möjligheterna att utveckla MI till ett användbart planeringsverktyg för att förebygga kemikalieolyckor visade sig goda. Valet av ett representativt set av kemikalieolyckor gjordes med hjälp av statistisk multivariat design (PCA) och baserades på ett insamlat set med 55 kemikalieolyckor av skiftande karaktär. De 18 valda olyckorna representerar därmed ett brett spektra av kemikalieolyckor. För att utveckla ett mått på miljöeffekt av en kemikalieolycka så användes en expertpanel som ombads att bedöma miljöeffekter (ex effekt på djurliv i vatten och markmiljön) av de utvalda kemikalieolyckorna. Resultatet visade att experternas bedömningar ger en god skattning av miljöeffekter av kemikalieolyckor och att de kan användas i utvecklingen av MI. För att förbättra MI relaterades responserna till de kemikalie- och områdesspecifika egenskaperna med hjälp av multivariat modellering (PLS) och en ny MI modell togs fram, tillsammans med en ny klassificeringsskala. Fördelarna med det nya MI jämfört med det gamla är att det nya MI kan beräknas utan att behöva använda tabeller, det kan skatta miljöeffekter för de ingående responserna och klassa kemikalieolyckor enligt den nya klassificeringsskalan. Slutligen så är det nya MI mer pålitligt att användas än MI eftersom det är byggt på ett set av representativa kemikalieolyckor och därmed också täcker ett bredare spektra av olycksscenarier. I det fortsatta arbetet med det nya MI kommer följande områden att prioriteras; att genomföra en extern validering av MI; att färdigställa formelstrukturen; att justera den nya klassificeringsskalan och att göra en verklighetsbaserad validering av MI.

**Nyckelord** Miljöolycksindex, kemikalieolyckor, miljöeffekter, frågeformulär, expertbedömningar, statistisk multivariat design, PCA, PLS

## Contents

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|   |           |
|---|-----------|
| List of papers.....   | <i>i</i>  |
| Abbreviations.....  | <i>ii</i> |
| 1 Introduction.....   | 1         |
| 1.1 Background and history.....   | 1         |
| 1.2 The situation today.....  | 2         |
| 1.3 Existing models – a review.....   | 4         |
| 1.3.1 The chemical risk database.....                                       | 5         |
| 1.3.2 Risk Index Z.....   | 6         |
| 1.3.3 Chemical exposure index (CEI).....                                    | 7         |
| 1.4 Description of the originally presented Environment-Accident Index..... | 8         |
| 1.5 EAI and the risk management process.....                                | 11        |
| 1.6 About this thesis.....  | 12        |
| 1.7 Aim.....  | 14        |
| 2 Chemical accidents.....   | 15        |
| 2.1 Assembling data on chemical accidents.....                              | 15        |
| 2.2 Dataset of chemical accidents – example of accidents.....               | 17        |
| 2.3 Properties describing the accidents.....                                | 19        |
| 2.3.1 Chemical property variables.....                                      | 19        |
| 2.3.2 Site-specific variables.....  | 20        |
| 2.4 Expert panel judgements of selected accidents.....                      | 21        |
| 3 Multivariate methods and Statistical design.....                          | 24        |
| 3.1 PCA.....  | 24        |
| 3.2 PLS.....  | 26        |
| 3.3 Validation of models in PCA and PLS.....                                | 28        |
| 3.4 Statistical design.....   | 29        |
| 4 Initial evaluation of the EAI.....  | 31        |
| 4.1 Stage I - test of EAI on chemical accidents.....                        | 31        |
| 4.2 Stage II - theoretical test.....  | 38        |
| 5 Selection of a representative set of chemical accidents.....              | 41        |
| 5.1 Selection procedure.....  | 41        |
| 5.2 Results of the selection.....   | 43        |
| 6 Estimating environmental effects using expert judgements.....             | 46        |
| 6.1 Results of the judgements.....  | 49        |
| 6.2 Summary.....  | 55        |
| 7 Relating accident descriptors to expert judgements.....                   | 56        |
| 7.1 PLS modelling.....  | 57        |
| 7.2 $EAI_{new}$ in relation to $EAI_{old}$ .....                            | 59        |
| 7.3 Classes.....  | 61        |
| 7.4 Observed vs predicted effects.....                                      | 62        |
| 7.5 Prediction of responses for 37 chemical accidents.....                  | 63        |

|     |  |    |
|-----|--|----|
| 7.6 | Practical use of EAI <sub>new</sub> .....                        | 65 |
| 7.7 | Summary.....   | 66 |
| 8   | Interviews .....   | 68 |
| 8.1 | Background.....  | 68 |
| 8.2 | Has the view of chemical accidents changed over the years? ..... | 69 |
| 8.3 | Organisation related to chemical accidents .....                 | 69 |
| 8.4 | Equipment.....   | 70 |
| 8.5 | How well are the accidents managed?.....                         | 71 |
| 8.6 | Evaluation of accidents and use of external experts .....        | 71 |
| 8.7 | Preventative work and cooperation .....                          | 72 |
| 8.8 | Further education, practical tools and lessons learned.....      | 73 |
| 8.9 | The role of the responsible authorities.....                     | 74 |
| 9   | Concluding remarks and future perspectives .....                 | 75 |
| 9.1 | Future work.....   | 78 |
| 10  | Acknowledgements .....   | 80 |
|     | References .....   | 82 |
|     | Appendix I-III .....   | 95 |

## List of Papers

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This thesis is based on the following papers, which will be referred to by their roman numerals.

- I. Scott Å, Environment-Accident Index: validation of a model, *Journal of Hazardous Materials* 61 (1998) 305 – 312.
- II. Scott Å, Tysklind M, and Fångmark I, Selection of a representative set of chemical accidents from a complex data matrix for the development of environment-accident index. *Journal of Hazardous Materials* A91 (2002) 63-80
- III. Scott Å, Stjernström O, and Fångmark I, Questionnaires and Expert Panel as a method to judge environmental consequences from chemical spill for the development of Environment-Accident Index, Submitted to *Journal of Environmental Management* 2003.
- IV. Scott Å, Tysklind M, and Fångmark I, Relating chemical accident properties and expert judgements in order to derive useful information for the development of Environment-Accident Index, (Manuscript).

## Abbreviations

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|                |  |
|----------------|--|
| AHE            | Acute Hazardous Events Database  |
| Am             | Amount of chemical according to EAI <sub>old</sub>                     |
| EAI            | Environment-Accident Index   |
| Con            | Consistency i.e the Viscosity  |
| D              | Density  |
| DGS            | Distance to groundwater surface  |
| DNW            | Distance to nearest well, lake or watercourse                          |
| EHO            | Environmental Health Officer   |
| EHPD           | The Environmental Health Protection Department                         |
| EL             | Effect level %   |
| ERA            | Environmental Risk Assessment  |
| FACTS          | Database for accidents with hazardous materials                        |
| FRS            | The Fire and Rescue Service  |
| HA             | Hazard Analysis  |
| HRA            | Health Risk Assessment   |
| K'             | Adjusted hydraulic conductivity for each soil and chemical             |
| m              | Amount   |
| MARS           | Major Accident Reporting System  |
| MHIDAS         | Major Hazard Incident Database Service                                 |
| n              | Soil porosity  |
| P <sub>v</sub> | Vapour pressure  |
| PCA            | Principal component analysis   |
| PLS            | Partial least squares projections to latent structures                 |
| POP:s          | Persistent Organic Pollutants  |
| Q <sup>2</sup> | Cross-validated explained variance                                     |
| R <sup>2</sup> | Explained variance   |
| RA             | Risk Assessment  |
| RMP            | Risk Management Process  |
| S <sub>w</sub> | Water solubility   |
| SGS            | Slope of groundwater surface   |
| SGU            | Geological Survey of Sweden  |
| Sol            | Water solubility   |
| SP             | Spreading part   |
| SRSA           | The Swedish Rescue Services Agency                                     |
| Sur            | Properties of the surrounding environment i.e site specific properties |
| Tox            | Acute toxicity to waterliving organisms                                |
| TS             | Training set   |
| USEPA          | United States Environmental Protection Agency                          |
| v              | Viscosity  |
| VS             | Validation set   |

# 1 Introduction

---

## 1.1 Background and history

Many activities in modern society are connected to the production and use of man-made chemicals. After World War Two intensive work in chemical laboratories resulted in a dramatic increase in the synthesis and isolation of new chemical compounds. In 1942, a mere 600 000 chemical compounds were known. In 1947, this number had increased to 4 million and since then the total number of identified chemical compounds has risen to around 11 million (*Lönngren 1992*). At many stages during the production, transportation, storage and use of many of these chemicals there is a risk that accidents will occur, both the possibility of occurrence and the severity of possible accidents depending on the chemicals concerned.

The largest overall environmental impact of chemicals is due to diffuse and continuous discharges from human activities such as industry, transport and agriculture. These activities are also the most intensively investigated. Nevertheless, chemicals released through accidents and other sudden, isolated events also affect the environment (and human health).

Many severe chemical accidents in recent history have affected the environment (and humans). However, some of the recent include the Bhopal accident in India in 1984 (*Bowonder and Linstone 1987*), the Sandoz accident in Switzerland in 1986 (*Brüggemann and Halfon 1990*), the Exxon Valdez accident in Prince William Sound in Canada in 1989 (*Shaw 1992*), and finally the Seveso accident in Italy in 1976 (*Pocchiari and Silano G Zapponi 1986*). The release of dioxin from a plant near Seveso in northern Italy on June 10<sup>th</sup> 1976 had severe consequences for both the environment and human beings. This accident, and subsequent incidents, resulted in Council Directive 82/501/EEC, more commonly known as the Seveso Directive, following three years of negotiation in the European Council and European Parliament. This directive was reviewed and updated in 1996 resulting in the implementation of the Seveso II Directive (*Council Directive 96/82/EC*). The Seveso Directives are “..aimed at the prevention of major accidents which involve dangerous substances, and the limitation of their consequences for man and the environment, with a view to ensuring high levels of protection throughout the Community in a consistent and effective manner”.

The Seveso directives are mainly focused on major accidents, which according to the definition by the European Council in 1982 are “sudden, unexpected, unplanned events, resulting from uncontrolled developments during an industrial activity...cause serious immediate or delayed adverse effects... to a number of people...”. However, the impact of smaller accidents at a more regional and local level also has to be assessed since numerically they widely exceed the number of major accidents. Thus, smaller incidents can make significant contributions to the overall environmental impact of accidents. The amounts spilled in the accidents considered in this thesis mostly varied from 100 L to 15 m<sup>3</sup>, so they are regarded as relatively minor accidents.

## 1.2 *The situation today*

The complexity and increasing flow of chemicals has resulted in more rigorous demands being placed on both authorities and industrial facilities that handle chemicals to estimate the risks involved. Industry is responsible for taking appropriate measures to handle chemicals safely and the authorities are responsible for giving appropriate guidelines.

The authorities responsible for dealing with chemical accidents at a local level in Sweden are the Environmental and Health Protection Departments<sup>1</sup> (EHPD) and the Fire and Rescue Services<sup>2</sup> (FRS) of the 290 municipalities. Unless the accident is very large and complex, in which case other authorities could also be involved, personnel from the EHPD and the FRS are responsible for taking all the appropriate decisions. The chain of actions taken after a chemical accident varies somewhat between localities, depending on their administrative structures, but typically it may include the following sequence. An SOS alarm<sup>3</sup> notifies the FRS, which is usually the first authority to arrive at the accident site. Following the Swedish Rescue Services Act (*The Swedish Statute-book 1986:1102*) the FRS must respond to accidents in order to prevent and restrict damage to people, property and the environment. The EHPD is usually the second authority to send representatives to the accident site, and they are in charge as soon as the FRS personnel have completed their tasks. The EHPD is responsible for ensuring that the decontamination process is satisfactory accomplished. The

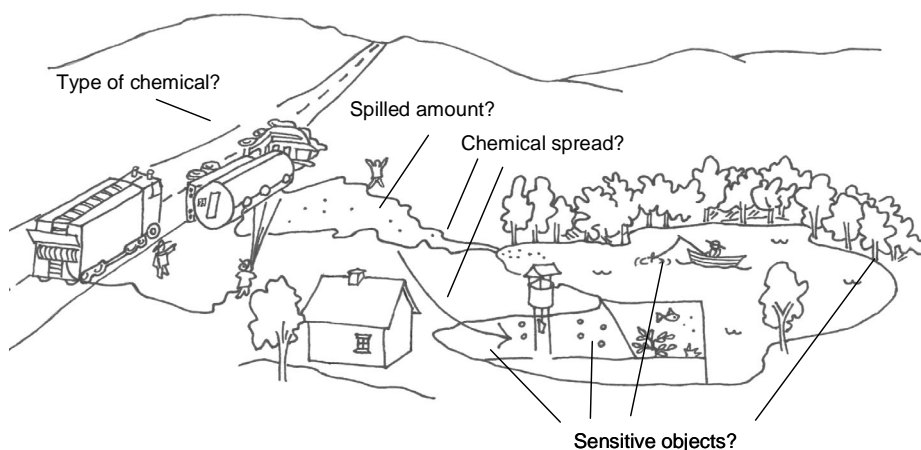
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<sup>1</sup> The EHPD is the municipal department responsible for ensuring that proper actions are taken to protect the environment in case of an accident.

<sup>2</sup> The FRS is the municipal fire department, and is responsible for the initial actions to protect humans, the environment and property.

<sup>3</sup> The Emergency Services Switchboard OR Regional Alarm Centre in Sweden

FRS takes the first damage-limiting measures and at the same time notifies the EHPD that the accident has occurred. In Sweden, the EHPD is not on emergency duty 24 h/day, unlike the FRS (except in one or two municipalities). The objective for the EHPD is to assess the potential hazards to the environment at the accident site and to make sure that proper actions are taken to limit damage. This quick assessment is based on information about both chemical and site-specific properties, including the likely spread and impact of the chemical. Figure 1 illustrates various factors that the FRS and the EHPD have to consider at an accident site. Some of these factors include: the type of chemical(s) involved, the amount spilled, the properties of the chemical, the likely routes and rapidity of its dispersal in the environment, its toxicity, and features that it may affect. Critical considerations are whether or not there are any especially sensitive objects in the area and the likelihood that they may be affected.



**Figure 1.** An accident site and factors to consider (after Hans Lundholm 1996)

Other important actors at the accident site may include staff from the facility that was handling the chemical (e.g. factory or chemical warehouse). In most cases these people have extensive knowledge about the chemicals and their behavior, and can thus give essential information about the environmental risks they pose. The industries involved are of course also responsible for the precautionary measures taken to avoid accidents and limit the damage in case of an accident.

Due to the number and wide range of existing chemicals it is unfeasible to assess the environmental effects of each and every one of them. Furthermore, data related to factors such as their toxicity, bioavailability, degradation and potential synergistic and antagonistic effects are only

available for a minor fraction of the chemicals. Thus, making a proper assessment of the environmental risks after a chemical accident is not straightforward.

According to the European Environment Agency (1998), other problems related to chemical accidents include the potential scale of their effects, their unpredictability and the uncertainties of their consequences. These problems, in combination with the lack of data and the complexity of the environment, make the task of environmental risk assessment (ERA) appear to be almost impossible. Therefore, tools such as indicators, indices and other models for ERA have been developed to assist and facilitate such assessment.

Risk assessment (RA) is not a new concept, although its application in a structured analytical format to environmental issues and policy is a relatively new development. Since the 1980s, ERA has not only advanced dramatically, but has also challenged the established views that science is inviolable and that experts are never wrong (*Eduljee 2000*). Although systems for ERA have been under development for several decades, problems such as lack of knowledge about chemicals' properties, their behaviour in the environment and site-specific properties, the complexity of the environment and the lack of a good system for assimilating lessons learned still need to be resolved.

### *1.3 Existing models – a review*

The literature review showed that the assessment of risks related to handling chemicals is a wide area that has been intensively researched. Generally, the models that have been developed can be divided into two groups: one concerned with long-term effects and the other with acute effects.

Models related to long-term effects cover the transport and fate of chemicals, often persistent organic pollutants (POP:s ) and heavy metals, following both instant and diffuse discharges of chemicals. The models include both human health risk assessments (HRA) and ecological or environmental risk assessments over long-term perspectives and consider persistency, degradation and bioaccumulation of the chemicals. One example is the fugacity model by Mackay (1991), describing the transport, distribution and fate of a chemical in different environmental compartments.

The group of models related to acute effects is the most interesting in the context of this thesis. It comprises models for both RA and ERA of chemicals, often combined with more general components for modelling the risk and consequences of instant spills of a chemical. These models are often designed to facilitate land-use planning, and the classification and/or ranking of chemicals and industrial facilities to facilitate the organisation of preventative measures. These models are generally based on inherent properties of the chemicals, rather than properties and characteristics of the accident site (surroundings). The literature review shows that there are currently three main models relevant to this thesis. These models, which are discussed below, are the:

- 1) Chemical risk database (*Ziegler 1992*)
- 2) Risk index Z (*Bello et al 1997*)
- 3) Chemical Exposure index (*Easterbrook 1988*)

### *1.3.1 The chemical risk database*

The chemical risk database, developed in Switzerland (*Ziegler 1992*) is a database for registering dangerous goods in a certain area (e.g. a city). The information in the database is used to make risk assessments of the current situation, mainly from a health risk perspective. From this assessment it should be possible to prioritise the risks from the most to the least acute, and thus take appropriate safety precautions. The advantage with this model is that it is possible to handle large amounts of data in a relatively short time. The first step in the assessment process, using the chemical risk database, is to define the area to be assessed. The second step is to collect data about relevant chemicals (individually, not in classes) and the amount of each chemical involved. The next step is to calculate the damage-potential for each chemical, which depends on the amount and toxicity of the chemicals, and will always be the same for each specific chemical, regardless of the surrounding environment. The potential damage occurs only when the chemical is related to an accident scenario. Six accident scenarios are defined, based on the nature of the causal events spill, fire, explosion and flooding. A computer program, C-RISK handles the large amount of information generated, and calculates the damage potential automatically.

### ***Comments on the model:***

The model is aimed to provide an overview of the accumulated specific risks within an area and give some order of priority. The damage potential is a useful tool for making a relative assessment of the potential hazard within an area, e.g. one factory compared to another. This comparison makes it easy to decide where to place the most effort. However, the model is primarily focused on humans rather than the environment. One disadvantage with this model is that it is limited to the specific scenarios, and does not cover other types of accidents. The model also distinguishes between different types of chemical accidents, and is designed to consider releases to air and fire scenarios. The model is quite complex to calculate because of the many intermediate steps that need to be calculated and special software is required for the storage of data and computation involved. This can be disadvantageous for the distribution of the model to authorities and other actors, as they may regard the model as too complex and expensive to use.

#### ***1.3.2 Risk Index Z***

Risk Index Z or “Classification system of the substances endangering subsoil and groundwater quality: Criteria for the notification of major accidents and hazardous installations” was developed as part of an EU-project at the Joint Research Centre (JRC) in Ispra, Italy (*Bello et al 1997*). The model was created for the prevention of soil and groundwater damage due to chemical spills. The model considers the inherent properties of the chemical(s), such as their toxicity, viscosity and water solubility. Risk Index Z has three components: toxicity (T), mobility (M) and Persistence (P). The toxicity component is based on the R-phrases<sup>4</sup>, which are already in use within the EU, the mobility component includes terms for density,  $\log K_{oc}$ <sup>5</sup> and vapour pressure as well as viscosity and water solubility. The properties are judged according to different tables and assigned an index number. The different indices are then summarised and assigned a mobility class (less, moderate or very mobile), and different classes have different mobility indices. Finally, the persistency component assesses abiotic, anaerobic and aerobic degradation, and the different degradation paths are assigned different index numbers.

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<sup>4</sup> Regulations according to directives 67/548/EEC (substances) and 1999/45/EC (preparations) stipulate that chemical products that are dangerous to health or the environment are to be labelled with appropriate risk-phrases (R-phrases) and symbols.

<sup>5</sup>  $\log K_{oc}$  is the partitioning coefficient between soil and water normalised to organic carbon content (oc).

The Risk Index Z is the product of the three partial indices, T, M and P:

$$\text{Risk Index } Z = T \cdot M \cdot P$$

The index is then classified on a four-grade risk scale (classes 0-III).

***Comments on the model:***

This model is interesting as it is the only index-based model available that is focused on the environment. However, the model is probably developed rather for describing long-term effects than acute effects in the environment. The assessment of the toxicity is based on the R-phrases, which might be a good approach as long as there are expressions for all the types of chemicals that may be involved. The mobility component seems to be relatively thoroughly assessed because the sorption and retention of the chemicals are considered as well as more obviously mobility-related factors. The persistency component considers both abiotic and biotic degradation pathways, indicating a focus on long-term perspectives. The Risk Index, Z, can be used to make assessments of mixtures as well as pure compounds, but it does not consider synergistic or antagonistic effects. The disadvantages with the model are that site-specific properties and the spilled amount of the chemical are not included in the index, and must therefore be considered afterwards, together with the derived risk index. The model is probably quite complicated to use, and another concern is that R-phrases and degradation data are only available for a limited number of chemical compounds.

***1.3.3 Chemical exposure index (CEI)***

CEI is a relatively old Canadian model (*Easterbrook 1988*), which ranks the health risk of an acute spill of a chemical to air. CEI is based on the following five factors, all of which can affect the level of exposure from a potential spill.

- I. **Toxicity:** the EEPG (Emergency Exposure Planning Guide value) concentration is multiplied with the pressure 760 mm Hg and then divided by the vapour pressure for the specific chemical.
- II. **Amount:** the maximum amount of a compound that can be vaporized during a 15 minutes release in a “worst case” situation.

- III. **Distance:** given as the distance in metres or kilometres to habitations, churches, schools, hospitals, hotels and shopping centres etc.
- IV. **Molecular weight:** the molecular weight of a chemical is directly related to its vapour density.
- V. **Process variables:** factors that can affect the size of the vapour cloud such as temperature, pressure and reactivity.

The different factors (I-V) are assigned values according to an internal scale and then the CEI is calculated:

$$CEI = I \cdot II \cdot III \cdot IV \cdot V$$

All factors have equal weight in the CEI except for toxicity, which is given a higher internal weighting. CEI focuses on the level of measures that should be implemented under given scenarios, and provides scope to create recommendations and to initiate communication between actors who will be involved in dealing with specific incidents.

#### ***Comments on the model:***

The CEI has two interesting features, even if it is focused on the effects on humans of releases to air rather than environmental effects. The molecular weight may be of interest, as it can also affect the spread of a chemical in the soil environment. Another interesting feature of the CEI is that it is a product of a range of factors, each of which is given equal importance in the calculation. Furthermore, only the internal weight of each factor has to be considered.

#### *1.4 Description of the originally presented Environment-Accident Index*

In our society, strenuous efforts have been made to develop different models to predict the possible environmental consequences of chemical spills. However, the majority of these models do not attempt to combine site-specific variables (e.g. soil and water variables) with inherent properties of the chemicals, (e.g. toxicity, density and volatility), but focus only on the chemicals *per se*, and their inherent capacity to harm the environment. However, the Environment-Accident Index (EAI) is an exception, since the rationale for its development was to obtain an assessment tool combining properties of the chemicals with site-specific properties.

The EAI was initially proposed by Fisher *et al* (1995). This model, derived from a template suggested by Nüßlein *et al* (1994), was deliberately formulated as a simple equation in order to facilitate and increase its applicability. The objective of the EAI is to provide a quick and simple tool to guide the identification and ranking of chemical accident scenarios in a planning process. The EAI can indicate the kind of further assessment that should be performed and what predictive measures should be taken for each specific scenario. The EAI can be used in planning processes by both appropriate authorities (especially the EHPD and the FRS), and industrial concerns that handle chemicals.

The EAI is based on a few chemical variables and site-specific variables such as soil and groundwater conditions (Eq. 1). It consists of three components: the acute toxicity to water-living organisms, represented by **Tox**; the stored or transported amount of the chemical, represented by **Am**; three factors affecting the spread of a chemical (**Con**, **Sol** and **Sur**). **Con** is the consistency or viscosity/physical state of the chemical, **Sol** is the water solubility of the chemical while **Sur** describes its potential to penetrate soil, together with the depth and mobility of groundwater.

$$\text{EAI} = \text{Tox} \cdot \text{Am} \cdot (\text{Con} + \text{Sol} + \text{Sur}) \quad (\text{Eq.1})$$

Each of the four variables **Am**, **Tox**, **Con** and **Sol**, is assigned a value according to Tables 6-9 based on the raw data (Appendix I).

In more detail, **Sur** expresses the properties of the surrounding environment (site-specific properties) in terms of

- 1) Distance, in metres, to the nearest well, watercourse or lake
- 2) Depth to the groundwater in metres
- 3) Whether the groundwater surface is inclined towards a well, lake or watercourse or if it is horizontal
- 4) The thickness, in metres, of the soil and the material it consists of, for example gravel, sand, moraine, silt, clay or frozen ground.

Each of the above four surrounding variables is assigned a value according to Tables 1-4 in Appendix I, and the sum is calculated. This sum gives, according to Table 5 in the same appendix, a value for the variable **Sur**. All contributing values are then included in the formula from which the EAI can be calculated.

What is not immediately apparent from the formula is that all variables have been weighted and transformed through use of the tables in Appendix I.

During the construction of the EAI, variables Con and Sol were given less weight (by a factor of around 0.5) in the tables compared to the other variables, i.e. Am, Tox and Sur.

After the EAI has been calculated, it can be used to identify the level of risk assessment required for a given scenario according to a set classification scale (*Fisher et al 1995*). The classification scale was constructed to facilitate the ranking and prioritisation of different accident scenarios to help prevent chemical accidents or to limit damage following an accident. Three classes, with different levels of action to be taken, were considered sufficient to spread the accident scenarios.

*Three-graded classification scale to determine the need for further risk assessment:*

|                      |  |
|----------------------|--|
| <b>EAI: 0-100</b>    | Hazard Analysis (HA) concerning the inherent properties of the chemical should be performed <sup>6</sup> |
| <b>EAI: 100-500</b>  | HA + <i>Introductory ERA</i> should be performed <sup>7</sup>  |
| <b>EAI: &gt; 500</b> | HA + <i>Introductory ERA</i> + <i>Advanced ERA</i> should be performed <sup>8</sup>                      |

The EAI is specifically related to Swedish organizations in terms of the agents involved and the recommended actions. Nevertheless, this does not hinder its implementation and use in countries with different administrative structures for handling chemical accidents.

EAI is valid for discharges to ground, water or groundwater but it is not applicable to fires, explosions or accidents in which gases are released to the air. EAI can be used to assess the acute phase of an accident. Further, it can be applied to certain positions along a transport route as a particular location can be considered to have the same conditions as a permanent establishment, e.g. an industrial site. However, the EAI cannot be applied to entire transport routes, as such uses also require the consideration of probability aspects.

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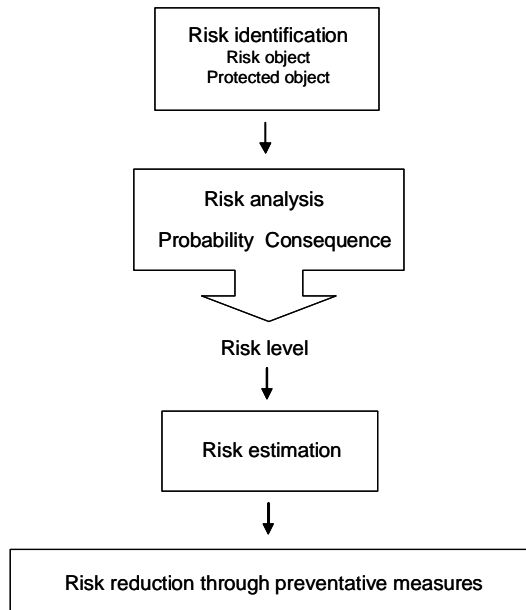
<sup>6</sup> Hazard Analysis is here defined as an overall assessment of inherent chemical properties, such as data on chemical and physical properties, mobility, degradation, toxicity and environmental risk phrases. Identification of where in the environment the chemical may accumulate, and how long the environmental effects might last is also involved.

<sup>7</sup> Introductory EAI is here defined as an expanded form of Hazard Analysis, including data on the present site of chemical handling.

<sup>8</sup> Advanced ERA is here defined as a comparison between the Predicted Environmental Concentration (PEC) and the Predicted No Effect Concentration (PNEC), and since an accident is often of short duration, the acute toxicity is used to calculate PEC. If  $PEC > PNEC$  there is a high risk of environmental effects, while if  $PEC < PNEC$  the risk is low.

### 1.5 EAI and the risk management process

EAI is a tool to facilitate the planning process with respect to the environmental consequences of chemical accidents, but how does the EAI fit into the risk management process (RMP)? In Figure 2 the steps in a risk management process (*Swedish Rescue Services Agency 2001*) are briefly described.



**Figure 2.** Steps in the risk management process

Firstly, the risk identification step involves identifying the risk object (e.g. industrial site or transportation of dangerous goods) and the protected object (e.g. pollution-sensitive areas, water supply plants, hospitals and schools). Secondly, during the risk analysis phase the probability that an accident will occur and the consequences of an accident are calculated. The risk analysis can be either qualitative or quantitative, deterministic or probabilistic. Qualitative risk analysis is used when the aim is merely to identify risk scenarios, and quantitative analysis when it is important to estimate the size of the risk (i.e. to calculate the probability and consequences of accidents). In deterministic analyses, which are based on accidents and their consequences, worst case scenarios and dimensioned casualty (i.e. damage that has been reduced by appropriate measures) are commonly used. Probabilistic or risk based analysis is based (except for the consequence components) on the probability that an accident will occur. Thirdly, the risk analysis generates risk levels that will be considered in the risk estimation

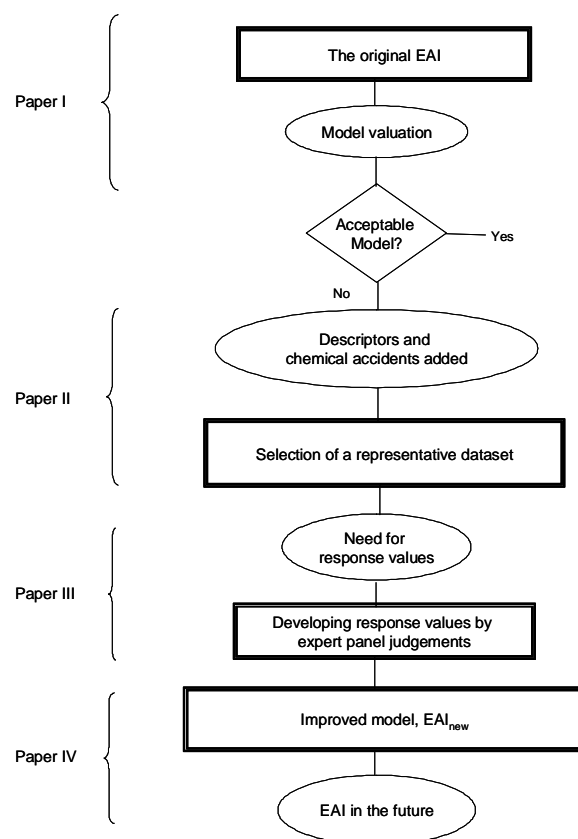
step. Finally, the process leads to proposals for preventative measures to lower the risk levels.

In order to see how the EAI approach is related to the classical risk management process a stepwise comparison can be made. The EAI and RMP are identical in terms of identifying risks (the object and features to be protected), but in the analysis step the EAI is based solely on a deterministic rather than a probabilistic approach. In the analysis step, using EAI, any scenario with a chemical spill can be considered, and a number of specific input parameters are fixed. In RMP, the analysis step involves methods for calculating frequencies (probabilities) and models for calculating consequences presented as risks for both individuals and society. The output of the EAI analysis is an index value that indicates the kind of further risk assessment that should be made, and the preventative measures that should be taken. In the RMP analysis the calculated output will be used to develop a preventative measures proposal. Thus, the risk estimation steps of the EAI and RMP approach are also similar, but the methods used in the risk analysis steps differ.

### *1.6 About this thesis*

Predicting the environmental consequences of a chemical accident is an extremely complex task. However, it is more important to be able to foresee the environmental consequences of chemical accidents in order to take appropriate precautionary actions. The EAI was developed to assist authorities and industrial concerns in their preventative work. It is therefore important for it to be user-friendly. The criteria for a useful index used here are that it should be based on simple and easily calculated equations, yet provide a tool that can both roughly classify accidents, covering a broad spectrum of accident scenarios, and give rough estimations of environmental effects.

An important step in the development of the index was to make an independent, but systematic selection, of a set of accidents to include in the development process, to avoid creating a biased model that was only applicable to a limited range of chemical accidents. In the work described in this thesis, the various steps in the development of the EAI have been evaluated, and the different steps in the development of the EAI are presented in Figure 3. The EAI is focused on organic chemicals and limited to fixed installations where a specified spot along a road can also be regarded as a fixed installation.



**Figure 3.** EAI – the development process and an overview of the papers presented in this thesis

The first test of the EAI and the included variables was based on 21 chemical accidents (Paper I). After the first valuation, data on additional accidents were included, new describing variables were added and representative training and validation sets were selected (Paper II). The third paper (Paper III) deals with the development of response values using questionnaires and expert panel judgements. Finally, the response variables and the descriptor variables of the chemical accidents are modelled together in Paper IV. The objective was to analyse the importance and weight of the descriptor variables and to use the new knowledge in the creation of a new EAI formula.

### *1.7 Aim*

The general aim of the work described in this thesis was to develop a better EAI model according to the criteria described above by:

- Investigating the feasibility of the EAI approach.
- Selection of a representative set of chemical accidents.
- Analysing the usefulness and importance of the variables describing a set of representative chemical accidents.
- Developing response variables.

## 2 Chemical accidents

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### 2.1 *Assembling data on chemical accidents*

When the EAI was initially evaluated (Paper I), data on 21 chemical accidents (19 from Sweden and two from Finland) were assembled, mainly from accident reports, notes and newspapers (this material is described in a special section of the reference list) and these were the only useful accidents found during the six-month evaluation period. After the initial evaluation it was decided that more accident data needed to be included in the development process. Therefore, further material on chemical accidents had to be assembled.

Assembling information about chemical accidents with significant consequences for the environment was difficult. The main problem is not that there are no reports about such accidents, but that their environmental consequences have not attracted much publicity. Therefore, the accidents causing environmental effects have not been as intensively investigated and reported as accidents with adverse consequences for human beings. Another problem was that if an accident relevant to this project was found it was sometimes difficult to investigate it because there was no information on where to ask for additional data related to it.

Additional material on chemical accidents was initially sought both worldwide and within Sweden, and various databases were searched. In the 1980:s, several databases and reporting systems were developed in the post-Seveso Directive period. In Europe, the Major Accident Reporting System (MARS) database (*European Commission 1982; Drogaris 1993 and; Rasmussen 1996*), the FACTS database (*TNO, the Netherlands 1981 and 2001*), and the Major Hazard Incident Database Service (MHIDAS) have dominated this field (*Carson and Mumford 1988*), while in the US, the Acute Hazardous Events (AHE) database was developed by the US Environmental Protection Agency (*USEPA 1985*). Over the years these databases have grown in size; e.g. the MARS database contains data on more than 450 major accidents from the member states of the European Union, the FACTS database covers more than 16 000 accidents from all over the world, and the MHIDAS database more than 7000 accidents, predominantly from the UK and USA. However, these databases were developed to provide information on major accidents, focusing mainly on human health effects. At the time of their construction, most databases that hold information about chemical accidents, such as the MARS and AHE databases, were not meant to contain detailed information about the

environmental consequences of chemical accidents. Hence, fewer accidents with environmental consequences have been reported and the data on those that have been reported were generally insufficient for the purposes of this project.

These obstacles made it difficult to find the information needed for this study from existing databases. So how was the information on chemical accidents to be assembled? As the EAI is mainly aimed to facilitate planning for “normal” chemical accidents, i.e. types of accidents that are expected to be most frequent, the information was mainly sought at a local level in Sweden by means of an inquiry. For this purpose, inquiry forms were sent to the Environmental and Health Protection Departments (EHPD) and the Fire and Rescue Services (FRS) of all 289 municipalities in Sweden. The information asked for included a short description of the sites at which accidents had occurred, their cause, the chemical(s) involved (and the amount of the stored or transported chemical), followed by the potential damage caused to the environment. In this way, an enlarged database consisting of data on 42 additional accidents was assembled. These 42 accidents were then investigated more thoroughly, to gain more detailed knowledge about the chemicals involved, the location of the accidents and, if possible, lessons learned.

The selection process (Paper II) revealed that it was impossible at this stage to develop a single model including both organic and inorganic chemicals. This was because the variables describing the chemical properties of organic and inorganic chemicals were so different that they separated the dataset used for the selection into two groups in the model. Hence, a model including both organic and inorganic chemicals based on these variables would lose precision. Therefore, the study was limited to accidents with organic chemicals, and only 16 of the original 21 accidents could be used. Thus, the set of chemical accidents from which the training and validation set was selected (Paper II) contained information on 58 accidents (16 original, and 42 further accidents). In addition, three accidents (nos. 6, 7 and 52) were excluded from the set because they involved chemicals with an unusually high viscosity, which would have created an unbalanced design (see Paper II), leaving 55 accidents in the dataset.

## 2.2 Dataset of chemical accidents – example of accidents

The assembled dataset with 55 accidents (which occurred between 1986 and 1999), described by 10 variables<sup>9</sup>, is shown in Table 1.

**Table 1.** The assembled set of chemical accidents The removed accidents (nos 6, 7 and 52) are coloured grey in the table.

| No: | Chemical:                   | CAS-no:    | $P_v$ | $v$ : | $D$ : | $Sw$ : | $m$ :  | $Tox$ : | $m/Tox$  | $DNW$ : | $DGS$ : | $SGS$ : | $K'$ : | $n$ : |
|-----|-----------------------------|------------|-------|-------|-------|--------|--------|---------|----------|---------|---------|---------|--------|-------|
| 1   | Kerosene/Jet fuel           | 8008-20-6  | 0,1   | 1,5   | 808   | 0,1    | 10     | 3,1     | 3,20E+09 | 6       | 2       | 1       | 1      | 55    |
| 2   | Kerosene/Jet fuel           | 8008-20-6  | 0,1   | 1,5   | 808   | 0,1    | 22,6   | 3,1     | 7,30E+09 | 3       | 0,6     | 0,5     | 1      | 55    |
| 3   | Kerosene/Jet fuel           | 8008-20-6  | 0,1   | 1,5   | 808   | 0,1    | 24,2   | 3,1     | 7,80E+09 | 15      | 1,5     | 1       | 3      | 35    |
| 4   | Kerosene/Jet fuel           | 8008-20-6  | 0,1   | 1,5   | 880   | 0,1    | 38,8   | 3,1     | 1,30E+10 | 5       | 0,01    | 1       | 1      | 15    |
| 5   | Petroleum liq               | 115-86-6   | 0,1   | 9,5   | 880   | 0,1    | 88     | 100     | 8,80E+08 | 5       | 0,5     | 1       | 1      | 15    |
| 6   | Petroleum liq               | 8012-95-1  | 0,1   | 95    | 919   | 0,1    | 0,047  | 100     | 4,70E+05 | 17,5    | 2       | 0,1     | 1      | 15    |
| 7   | Heating oil No5             | 64741-45-3 | 1     | 41    | 965   | 0,1    | 483    | 55      | 9,90E+09 | 10      | 10      | 1       | 3      | 33    |
| 8   | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 328    | 2,6     | 1,30E+11 | 1       | 1,5     | 1       | 3      | 35    |
| 9   | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 24,6   | 2,6     | 9,50E+09 | 100     | 5       | 1       | 3      | 35    |
| 10  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 42,6   | 2,6     | 1,60E+10 | 9       | 3       | 1       | 1      | 55    |
| 11  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 9,84   | 2,6     | 3,80E+09 | 50      | 2       | 0,5     | 2      | 35    |
| 12  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 8,2    | 2,6     | 3,20E+09 | 3       | 1,5     | 1       | 1      | 15    |
| 13  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 4,2    | 2,6     | 1,60E+09 | 15      | 4       | 1       | 1      | 15    |
| 14  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 1,3    | 2,6     | 5,00E+08 | 3       | 6       | 0,5     | 1      | 43    |
| 15  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 24,6   | 2,6     | 9,50E+09 | 5       | 0,2     | 1       | 1      | 15    |
| 16  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 37     | 2,6     | 1,40E+10 | 7       | 0,35    | 1       | 1      | 15    |
| 17  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 49     | 2,6     | 1,90E+10 | 15      | 2       | 1       | 2      | 35    |
| 18  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 240    | 2,6     | 9,20E+10 | 220     | 4,4     | 1       | 2      | 35    |
| 19  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 0,5    | 2,6     | 1,90E+08 | 600     | 0,01    | 1       | 3      | 33    |
| 20  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 0,122  | 2,6     | 4,90E+07 | 1600    | 3       | 1       | 1      | 15    |
| 21  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 13,1   | 2,6     | 5,00E+09 | 5       | 8       | 1       | 1      | 55    |
| 22  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 4,9    | 2,6     | 1,90E+09 | 1       | 3       | 1       | 1      | 43    |
| 23  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 0,326  | 2,6     | 1,30E+08 | 2000    | 6       | 0,1     | 1      | 43    |
| 24  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 24,6   | 2,6     | 9,50E+09 | 350     | 3       | 1       | 1      | 43    |
| 25  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 4075   | 2,6     | 1,60E+12 | 13      | 7,2     | 1       | 3      | 33    |
| 26  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 0,8    | 2,6     | 3,10E+08 | 40      | 2       | 1       | 2      | 35    |
| 27  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 0,122  | 2,6     | 4,70E+07 | 0,01    | 1       | 1       | 1      | 15    |
| 28  | Diesel fuel/heating oil No1 | 68334-30-5 | 0,5   | 2,75  | 820   | 0,1    | 8      | 2,6     | 3,10E+09 | 17      | 13      | 1       | u      | u     |
| 29  | Gasoline                    | 86290-81-5 | 70    | 1     | 750   | 0,01   | 16,5   | 4,9     | 3,40E+09 | 3       | 3       | 1       | 1      | 43    |
| 30  | Gasoline                    | 86290-81-5 | 70    | 1     | 750   | 0,01   | 28,5   | 4,9     | 5,80E+09 | 25      | 0,01    | 1       | 2      | 35    |
| 31  | Gasoline                    | 86290-81-5 | 70    | 1     | 750   | 0,01   | 38,2   | 4,9     | 7,80E+09 | 100     | 0,01    | 1       | 3      | 33    |
| 32  | Gasoline                    | 86290-81-5 | 70    | 1     | 750   | 0,01   | 35,3   | 4,9     | 7,20E+09 | 2       | 16      | 1       | 1      | 43    |
| 33  | Gasoline                    | 86290-81-5 | 70    | 1     | 750   | 0,01   | 0,75   | 4,9     | 1,50E+08 | 8       | 2       | 0,5     | 1      | 15    |
| 34  | Gasoline                    | 86290-81-5 | 70    | 1     | 750   | 0,01   | 26     | 4,9     | 5,30E+09 | 0,01    | 12      | 1       | 1      | 15    |
| 35  | Gasoline                    | 86290-81-5 | 70    | 1     | 750   | 0,01   | 35,5   | 4,9     | 7,20E+09 | 2       | 1,87    | 0,5     | 1      | 43    |
| 36  | Gasoline                    | 86290-81-5 | 70    | 1     | 750   | 0,01   | 12     | 4,9     | 2,40E+09 | 9       | 8       | 0,1     | 1      | 15    |
| 37  | Gasoline                    | 86290-81-5 | 70    | 1     | 750   | 0,01   | 22,5   | 4,9     | 4,60E+09 | 200     | 6       | 1       | 1      | 15    |
| 38  | Gasoline                    | 86290-81-5 | 70    | 1     | 750   | 0,01   | 35,3   | 4,9     | 7,20E+09 | 100     | 9,4     | 1       | 2      | 35    |
| 39  | Gasoline                    | 86290-81-5 | 70    | 1     | 750   | 0,01   | 18     | 4,9     | 3,70E+09 | 7       | 2,6     | 1       | 1      | 15    |
| 40  | Gasoline                    | 86290-81-5 | 70    | 1     | 750   | 0,01   | 33,6   | 4,9     | 6,90E+09 | 7       | 5       | 1       | 1      | 15    |
| 41  | Methanol                    | 67-56-1    | 12,8  | 0,8   | 790   | 90     | 35     | 13200   | 2,70E+06 | 125     | 33      | 1       | 1      | 55    |
| 42  | Isopropanol                 | 67-63-0    | 4,2   | 3     | 790   | 90     | 0,18   | 2285    | 7,90E+04 | 300     | 2       | 1       | 2      | 35    |
| 43  | Benzene                     | 71-43-2    | 10,1  | 1     | 880   | 1,8    | 1232   | 5,3     | 2,30E+11 | 3       | 2       | 1       | 3      | 35    |
| 44  | Chlorobenzene               | 108-90-7   | 1,2   | 1     | 1110  | 0,05   | 1000   | 4,7     | 2,10E+11 | 30      | 2,3     | 1       | 1      | 15    |
| 45  | Phenol                      | 108-95-2   | 0,05  | 3,2   | 1070  | 8      | 90     | 3,3     | 2,70E+10 | 4       | 4,1     | 0,5     | u      | u     |
| 46  | Methyl methacrylate         | 80-62-6    | 3,7   | 2,25  | 940   | 1,5    | 47     | 159     | 3,00E+08 | 6       | 4       | 1       | 1      | 55    |
| 47  | n-Butylacetate              | 123-86-4   | 1,2   | 1     | 880   | 0,007  | 4,8    | 18      | 2,70E+08 | 25      | 23      | 0,5     | 3      | 33    |
| 48  | Vinyl acetate               | 108-05-4   | 12    | 1     | 930   | 0,02   | 29,8   | 18      | 1,70E+09 | 7       | 7,6     | 0,5     | 2      | 35    |
| 49  | Styrene                     | 100-42-5   | 0,6   | 0,9   | 910   | 0,01   | 60     | 9,1     | 6,60E+09 | 1       | 3,1     | 1       | 3      | 33    |
| 50  | 4-Chloro-m-cresol           | 59-50-7    | u     | 2,25  | 1370  | 0,001  | 0,002  | 7,6     | 2,60E+05 | 200     | 1,5     | 0,5     | 1      | 15    |
| 51  | Trichloroethylene           | 1979-01-06 | 7,7   | 0,9   | 1460  | 0,1    | 2      | 16      | 1,30E+08 | 30      | 7       | 1       | 3      | 35    |
| 52  | DEHP                        | 117-81-7   | vl    | 82,2  | 990   | 0,1    | 3,2    | 500     | 6,40E+06 | 30      | 1       | 1       | 3      | 33    |
| 53  | Benzenesulphonic acid       | 98-11-3    | u     | 2,25  | 1295  | 90     | 1,04   | 5,5     | 1,90E+08 | 15      | u       | 0,5     | u      | u     |
| 54  | Butylaldehyde               | 123-72-8   | 12    | 1     | 810   | 7      | 4,1    | 19      | 2,20E+08 | 35      | 3,2     | 0,5     | 1      | 55    |
| 55  | Formic acid                 | 64-18-6    | 4,3   | 1,5   | 1220  | 90     | 6,1    | 70      | 8,70E+07 | 30      | 3,2     | 0,5     | 1      | 15    |
| 56  | Glyphosate                  | 38641-94-0 | vl    | 2,25  | 1170  | 90     | 0,0157 | 86      | 1,80E+05 | 2       | 16,5    | 1       | 1      | 43    |
| 57  | Fluaziname                  | 79622-59-6 | vl    | 2,25  | 1300  | 0,01   | 0,0023 | 0,055   | 4,20E+07 | 5       | 3       | 1       | 2      | 35    |
| 58  | Metamitron                  | 41394-05-2 | u     | 2,25  | u     | 0,2    | 0,021  | 101,7   | 2,10E+05 | 100     | 4       | 1       | 1      | 55    |

For some chemicals the vapour pressure is very low and thus evaporation losses to air were considered negligible. Hence, the specific values for these

<sup>9</sup> The descriptor variables are: kinematic viscosity,  $\nu$  ( $\text{mm}^2/\text{s}$ ); water solubility,  $S_w$  (weight-%); amount,  $m$  (metric tonnes) of the stored or transported chemical; acute toxicity,  $Tox$  (mg/L); the ratio between amount and toxicity  $m/Tox$  (L); density  $D$  ( $\text{kg}/\text{m}^3$ ); vapour pressure,  $P_v$  (kPa); the distance to the nearest well, lake or watercourse,  $DNW$  (m); the depth to the groundwater surface,  $DGS$  (m); the slope of the groundwater surface and the flow direction,  $SGS$  (inclining towards a well lake or watercourse = 1, horizontal surface = 0.5 and no well lake or watercourse in the flow direction = 0.1); the hydraulic conductivity for each chemical and soil,  $K'$  (m/day); and porosity of the soil,  $n$ , (%).

chemicals were replaced with vl (very low) in Table 1. For some other accidents, information on the vapour pressure of the chemical, together with data on the hydraulic conductivity and porosity of the ground at the accident site, could not be found and were therefore labelled u (unknown). During the calculations, these entries were considered as missing data.

The dataset contained an over-representation of accidents with petroleum products (69%). This tendency was confirmed by statistics from the Swedish Rescue Services Agency (*Rescue operations 1996-1999*), which showed that 60-77% of chemical accidents that occurred between 1996 and 1999 involved petroleum products. Two examples of chemical accidents in the dataset are described below. The first was an accident involving heating oil that had major consequences for the drinking water supply.

*Example: Karlshamn, Sweden (accident15)*

In 1994 a transport accident occurred close to Karlshamn in Sweden. 12.3 tonnes of heating oil was spilled into Mieån (a small river), in the water catchment area for the municipality of Karlshamn. The water supply plant was shut off and water had to be temporarily drawn from a lake to provide the municipality with drinking water. After three months of restoration and decontamination Mieån could be used to supply drinking water again. 2.3 tonnes of heating oil was estimated to have been left in the environment.

The other accident, involving heated phenol, provides an example of potential consequences when some possible routes allowing the chemical to spread are either not known or are not considered.

*Example: Sundsvall, Sweden (accident 45)*

In 1986 a chemical accident occurred at a phenolic resin manufacturing plant. A valve on the emptying pipe from the stocking tanks, which at the time of the accident contained 47 m<sup>3</sup> of heated phenol, began to leak. The escaping phenol ran out of the embankment and spread out on the snow and ice covered asphalt. About 39 m<sup>3</sup> of phenol was discharged. The heated phenol melted the snow and was partly dissolved in the snow melt. The phenol/water mixture reached a forgotten clean-out well and via this dispersed further into the sewage system. The biological purification components in a downstream waste-water treatment plant were totally wiped out and the sewage system was contaminated. Two of the personnel at the plant had to go to hospital because of the fumes from the spill. The decontamination process took a month. 1000 kg of phenol was estimated to have been left in the environment.

### 2.3 *Properties describing the accidents*

The assembled dataset of chemical accidents was described by two groups of variables: one describing the chemical properties and the other describing the site-specific properties, as outlined in the following sections.

#### 2.3.1 *Chemical property variables*

The variables describing the chemical properties are: kinematic viscosity,  $\nu$ , water solubility,  $S_w$ , amount  $m$  of the stored or transported chemical, acute toxicity towards water-living organisms,  $Tox$ . Toxicity and amount are important variables for assessing effects on the environment. However, the toxicity associated with the amount released is the crucial factor governing the environmental effects of a chemical at an accident site. A weakly toxic chemical in large amounts can cause as much damage to the environment as a small amount of a highly toxic chemical. Therefore, the amount to toxicity ratio,  $m/Tox$  was calculated and used in the selection procedure. The water solubility of a chemical strongly affects both its dispersal properties and its toxicity towards the environment. The viscosity contributes to the (horizontal) spread of the chemical. As a result of the first validation, two new descriptor variables for inherent chemical properties were added to the data set, namely density,  $D$ , and vapour pressure,  $P_v$ . These new variables are important for describing the vertical transportation of the chemical in water and soil, together with evaporative losses to the air. The inherent chemical properties are given at 20°C.

Petroleum products are not pure compounds but mixtures of various hydrocarbons, and the toxicity, density, vapour pressure and viscosity values listed in the literature are given as intervals. It was therefore decided to use the arithmetic mean of the lowest and highest values.

The water solubility,  $S_w$  was used as follows: if the solubility was given as <1 wt%, the value 0.1 wt% was used, if the solubility was given as <<1 the value 0.01 wt% was used, and if the solubility was given as completely mixable or >90 wt%, the value 90 wt% was used.

The amount of the chemical used in the modelling is the maximal amount of the pure compound (or mixture) transported or stored. The reason for this is that a worst-case scenario should be used when calculating the EAI to avoid underestimating the situation. Therefore, mixtures with water were recalculated as if they were pure compounds.

Data on inherent chemical properties, such as viscosity, density and toxicity were collected from available literature. Properties related to the chemicals were gathered from various literature sources and databases such as BUA Report Series (1995), ChemFinder (1999), CONCAWE (*various reports from 1992-1998*), Hommel (1987), the Hazardous Substances Databank (*National Library of Medicine, USA 2000*), Environmental protection data sheets (*the Swedish Plastics and Chemicals federation 2000*), Dangerous goods cards (*the Swedish Fire Protection Association 2000*), and Environmental Properties of Chemicals (*Nikkunen et al 1991*). If information on one variable, e.g. toxicity was obtained from several sources, a worst case scenario was applied, e.g. in the case of toxicity the lowest value of LC<sub>50</sub> or EC<sub>50</sub> was used.

### 2.3.2 Site-specific variables

The properties of the surroundings were described by the distance to the nearest well, lake or watercourse, **DNW** (m), the depth to the groundwater surface, **DGS** (m), the slope of the groundwater surface and the flow direction, **SGS** (inclining towards a well, lake or watercourse = 1; horizontal surface = 0.5, inclining away from any well, lake or watercourse = 0.1) and the permeability of the soil. In the first validation, the permeability of the soil was expressed in terms of soil type, e.g. sand, gravel or clay. However, more quantitative variables were needed to better describe the behaviour of the chemicals in the different types of soils. Therefore, the type of soil was replaced by two new variables: the hydraulic conductivity for each chemical and soil, **K'** (m/day) and the porosity of the soil, **n**, (%). The calculated hydraulic conductivity values were calculated, assuming saturated soil conditions, according to Freeze and Cherry (1979):

$$K' = \nu_w / \nu' \cdot K_w \quad (\text{Eq. 2})$$

The variable  $\nu_w$  is the kinematic viscosity of water,  $\nu'$  is the kinematic viscosity of the chemical and  $K_w$  the hydraulic conductivity of water in the specific soil. The new variables give a better quantitative description of how a chemical will behave in the soil following a spill than merely using the type of soil together with the thickness of the specific soil layer.

The type of soil at an accident site is not always either clear or easy to judge. For instance, at industrial sites the soil may consist of fillings, which may be mixtures of many different materials. However, since fillings are

often highly permeable, they were regarded as sand or gravel in the calculations of hydraulic conductivity.

The hydraulic conductivity,  $K'$ , spanned several orders of magnitude, but it was considered precise enough to divide the data into three classes: 1 for values  $<1$  m/day, 2 for values of 1- 10 m/day and 3 for values  $>10$  m/day.

For the variable  $DNW$ , the ditches connected to watercourses were also considered, due to the risk of the chemical spreading further from ditches to larger watercourses or lakes. For accidents where the chemical was spilled directly into water,  $DNW$  was set to 0.01 m rather than 0, for transformation reasons.

Some of the data related to site-specific properties of each accident originate from unpublished material, such as accident reports, notes and oral information. These are therefore listed in a special section of the reference list. Data on the classification of soils regarding hydraulic conductivity and porosity are taken from Knutsson and Morfeldt (1978). For some of the accidents, where data could not be obtained from the accident reports, data on soil conditions were taken from the Geological Survey of Sweden (SGU) and data on wells and groundwater levels have been obtained from the Hydrogeological database HYDRODB (*Geological Survey of Sweden 2000*).

For accidents where no data were available on the depth to the groundwater surface, the mean  $DGS$  values of other accidents with known  $DGS$  values and similar types of soil were used to estimate their  $DGS$  values. For accidents where the chemical was spilled directly into water,  $DGS$  was set to 0.01 m rather than 0, again for transformation reasons.

In cases where data were lacking on variables that are not mentioned above, e.g. the thickness of the soil, the flow direction of groundwater etc., estimates have sometimes been used in calculations of the EAI.

#### *2.4 Expert panel judgements of selected accidents*

Various methods to obtain representative measurements of the effects in the environment of chemical accidents were evaluated. One such method is to use cell cultures to measure environmental effects, as explored by Leffler (2002) and Ragnvaldsson and Leffler (2001). In this method, mice cells are exposed to extracts from various types of soil polluted with various

chemicals, either from real accidental spills or “laboratory spills” and their effects on cell viability are measured. The method is based on industrial quality control techniques (*Andrén and Wieslander 1993*). This is an interesting approach that could be used in the future to gain additional knowledge about environmental effects and thus complement the present response variables. However, the data collection method used in studies reported in Paper III was a questionnaire designed for an expert panel to assess the environmental consequences of chemical accidents.

The panel consisted of environmental health officers<sup>10</sup> selected from a representative set of municipalities in Sweden. Environmental health officers were considered most qualified to make the judgements since i) they have the necessary education and experience and ii) they are currently the people who make these judgements in real chemical accident situations in Sweden.

The set of municipalities used for this purpose was selected from the existing 289 municipalities in Sweden according to the following strategy. A preliminary selection was based on the location of chemical plants (*the Swedish Plastics and Chemicals Federation 2001*) and statistics on the transportation of chemicals (*the Swedish Rescue Services Agency 1995*). This selection strategy was chosen because heavily industrialised areas generally have a higher frequency of chemical accidents. Thus, the people handling accidents in these municipalities gain more experience and should be more qualified to make sound judgements than their counterparts in other municipalities. The preliminary set consisted of 79 municipalities, from which 30 were selected randomly. Subsequently, the Environmental and Health Protection Administrations in these 30 municipalities were contacted by mail, followed by a phone call with a request to participate in the survey. 18 municipalities agreed to participate, and these were divided into two groups. One group of 10 experts were asked to judge the nine accidents in the training set, and the other group of eight experts judged the nine accidents in the validation set. During the judgement period one of the experts in the validation set was unable to complete the task, leaving the validation set with seven experts. A more detailed description of the selected municipalities can be found in Paper III.

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<sup>10</sup> Environmental Health Officers in Sweden work locally in the municipalities (the Environmental and Health Protection Department), and have a broad remit, covering diverse environmental matters, such as pollution, chemical spills, industrial environmental protection, food hygiene, food control, prevention of cruelty to animals, waste handling, drainage etc. The officers who participated in this study work daily with issues concerning chemicals, chemical spill and related fields.

The environmental health officers, hereafter called the experts, in the 18 municipalities were then given the questionnaires together with the accident summaries and a judgement period of four weeks was established. The experts were instructed to read each accident case, and then, after reading the questions in the questionnaire, to make their own judgement of the level of environmental damage on a scale varying from 0% (no effect) to 100% (very large effect).

The questionnaire consisted of two parts. The first dealt with the personal and professional background of the experts (Part I), while the second (Part II) asked about their assessments of the environmental effects (responses) of the selected chemical accidents.

The questions asked about each of the nine accidents in each set were related to their effects on: animal life and vegetation in the aquatic and terrestrial environment; water supplies; utilization of resources; and recreational facilities. A detailed description of the questions can be found in Chapter 6. Each question asked for judgements on a three-part time scale (1 day - 1 year, 1 - 5 years and >5 years), to assess short- to long- term effects.

Although the EAI is focused on acute effects, an extended time scale was set since it was important to find out if the experts were able to make such judgements. The experts were requested to quantify their judgements on a continuous scale, where 0% represented no effects, 25% represented small effects, 50% represented moderate effects, 75% represented large effects and 100% represented very large effects. The experts could choose to use either one of the given effect levels (i.e. 0, 25, 50, 75 or 100%), or any number between 0 to 100%.

### 3 Multivariate methods and Statistical design

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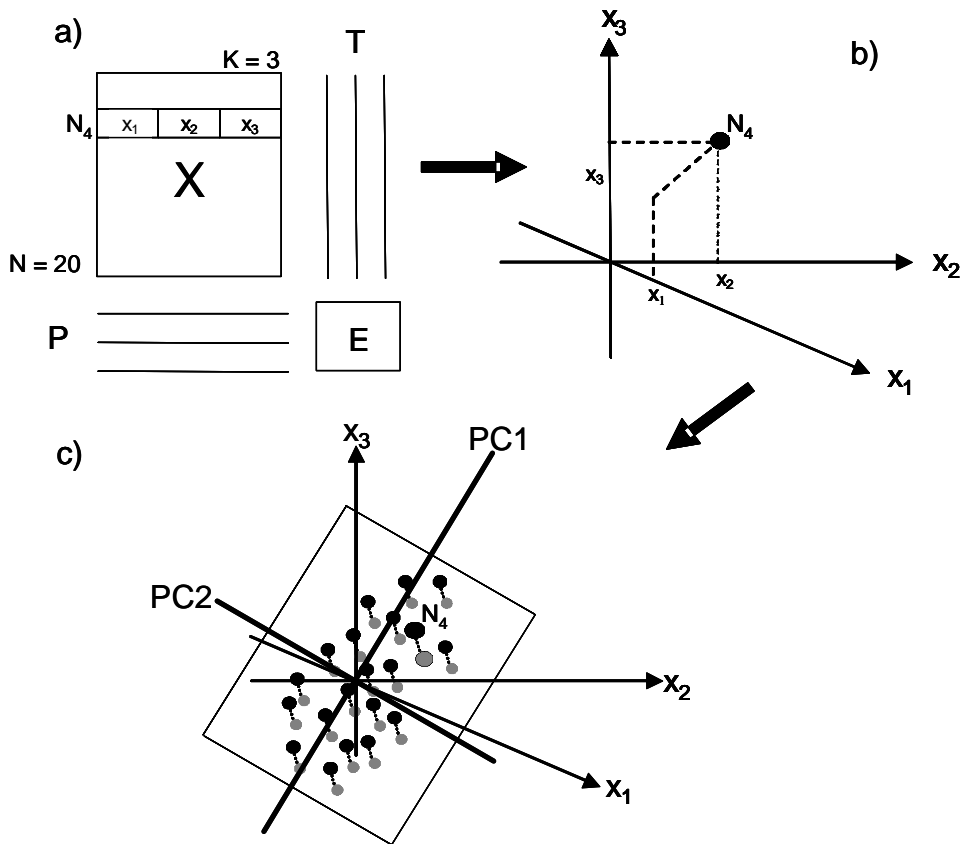
This Chapter outlines the data analysis tools used in the development of the EAI, namely Principal Component Analysis (PCA), Partial Least Squares Projections to latent structures (PLS) and statistical design. The advantage with these analytical tools is that they can handle co-linear and missing data in a satisfactory way.

#### 3.1 PCA

Generally, designed experiments provide the maximum amount of information. In this case the design must consider both the chemical properties and the site-specific properties (see Chapter 2 for further information). The experimental design should be done using independent variables. However, in the studies discussed in this thesis the property descriptors for the chemical and the surroundings for each accident are highly dependent. To overcome this problem, PCA was used to calculate new independent variables for each accident, which were then used as inputs in a statistical experimental design (see Section 3.4).

PCA is an analytical projection method that is designed to extract the systematic variation in large data tables and to get an overview of the data set with respect to all of the variables simultaneously, as described by Wold *et al* (1986) and Jackson (1991). As described by the cited authors, PCA can handle dependent descriptor variables, such as the group of chemical property variables used in this study. Figure 4 shows a schematic illustration of the method.

Thus, to ensure that a proper and unbiased selection of a representative set of accidents was chosen from the data set of 55 accidents, the data analysis method PCA was employed. This overview provided a basis for selecting a representative set of accidents for modelling and validating the EAI.



**Figure 4.** Illustration of the principles of PCA. (a) Dataset with  $N = 20$  objects (in this study 55 accidents) described by  $K = 3$  variables (in this study 10 chemical- and site-specific properties). (b) The location of object  $N_4$  in space is determined by variables  $x_1$ - $x_3$ , but the principal is the same even if  $K = 100$ . (c) In this case object  $N_4$  is projected onto a plane described by  $PC1$  and  $PC2$ . This plane is the best approximation of the 20 objects. The same procedure applies to all 20 objects.

Mathematically, PCA can be described as conversion of the data matrix  $X$ , in this case consisting of  $N = 55$  accidents (rows) and  $K = 10$  variables (columns), into a product of two smaller matrices  $T$  and  $P'$  (Figure 4a and Eq. 3), comprising object scores and variable loadings, respectively.  $E$  is the residual matrix and  $\bar{x}$  the row vector with variable averages (see Eq. 3).

$$\mathbf{X} = \mathbf{1} \cdot \bar{x} + \mathbf{T} \cdot \mathbf{P}' + \mathbf{E} \quad (\text{Eq.3})$$

From a data table with  $N$  objects described by  $K$  responses, each object can be represented as a point in a  $K$ -dimensional space defined by the  $K$  variables (Figure 4b). Accordingly, the data table will then constitute a swarm of points in the same space. PCA calculates linear combinations of the original  $X$ -variables to give a few orthogonal and independent

dimensions or principal components (PC:s) that summarise the dominant variation (directions) in the X-matrix. The first PC (PC1) will provide the best linear approximation of the matrix or swarm of points, PC2, the second best, and so forth. The PC:s form a line or hyperplane (depending on the number of significant PC:s) on which the objects are projected (Figure 4c). The results are displayed in two complementary plots to facilitate interpretation of the variation in the data. These plots are used to study relationships between objects (a score plot, described by score vectors  $t[1], t[2] \dots t[n]$ ) and between variables (a loading plot, described by loading vectors,  $p[1], p[2] \dots p[n]$ ). In the loading plot variables far away from the origin along PC1 are important for the horizontal distribution of objects in the score plot. Similarly, variables far away from the origin along the second PC are important for the vertical distribution of objects in the score plot. Outliers can be detected using Hotelling's  $T^2$  tool, which is a multivariate generalization of Student's t-test. Hotelling's  $T^2$  analysis can detect observations that are extreme or do not fit the PCA model well. In the score plots the Hotelling's  $T^2$  statistics define the normal area, by a tolerance ellipse, corresponding to, for example, a 95% or a 99% tolerance level. In this work the 95% level was used, meaning that  $N (=55 \text{ accidents}) \cdot 0.05 = 2.75$  observations (accidents) were expected to be outside of the ellipse.

### 3.2 PLS

To relate the descriptor variables of the chemical accidents (inherent chemical properties and site specific-properties) with the response values from Paper III a multivariate data analytical method, PLS, was used (Paper IV).

PLS is a data analysis technique that can handle data matrices with correlated variables like expert judgements, chemical properties etc. (Wold *et al* 1987). The method is also capable of handling large data matrices and it is better than traditional methods for handling noisy and missing data (Höskuldsson 1996; Eriksson *et al* 1999). PLS relates two data matrices: X (containing the properties of the chemicals involved and the site-specific properties of each accident) and Y (containing the responses, in this study the environmental consequences of each accident as judged by the experts) to each other. The method can be used to predict a response value,  $y$ , for a known set of  $x$ -variables. There are several similarities between PLS and PCA since the two techniques have the same theoretical foundations, both being based on principles of projection. Provided that the X- and Y-

matrices are measured on the same set of objects a PC-model with a few dimensions can give good approximations of both X and Y. PLS provides a way to compute these approximations so that the projections are as closely related to each other as possible. The computations are also performed in such a way that Y can be predicted from X.

PLS is built on a projection of each data matrix to latent structures where the correlation between the matrices is investigated. The new projected latent variables or vectors are calculated so that the first vector describes the highest correlation between X and Y, the second vector describes the second highest correlation and so on. The vector is a straight line through the average point of each point (observation) swarm that is fitted to the observations. Through projection of the points (observations) on this vector, the so-called score values are obtained and the score values of all observations form the first X-score vector  $t[1]$ . The same procedure is applied to the Y matrix, where the best correlation from Y to X is described with the first Y score vector,  $u[1]$ . Then vectors  $t[2]$  (always orthogonal to  $t[1]$ ) and  $u[2]$  (not necessarily orthogonal to  $u[1]$ ), can be calculated in the same way for maximum correlation.

Having done this,  $t[1]$  and  $u[1]$  are related to each other with the inner correlation,  $u_i[1] = t_i[1] + h_i$ , where  $h_i$  is the residual. After this, predictions can be made by inserting x-variables from an observation into the model and using the inner relation between  $t$  and  $u$  to predict the unknown y response value (Figure 5)

A PLS model may be re-expressed as a solution consisting of PLS regression coefficients, B, according to Eq. 4.

$$Y = XB \tag{Eq. 4}$$

Here, X refers to the X matrix, including squared and/or cross terms (if included), and Y is the response matrix. If X and Y are unscaled and uncentred, the regression coefficients are expressed as Eq. 5:

$$y_m = b_0 + b_1x_1 + \dots + b_kx_k \dots \text{etc} \tag{Eq. 5}$$

This solution has advantages when the purpose is to present the model to other people, who are not familiar with the latent way of thinking (*Eriksson et al 1999*).

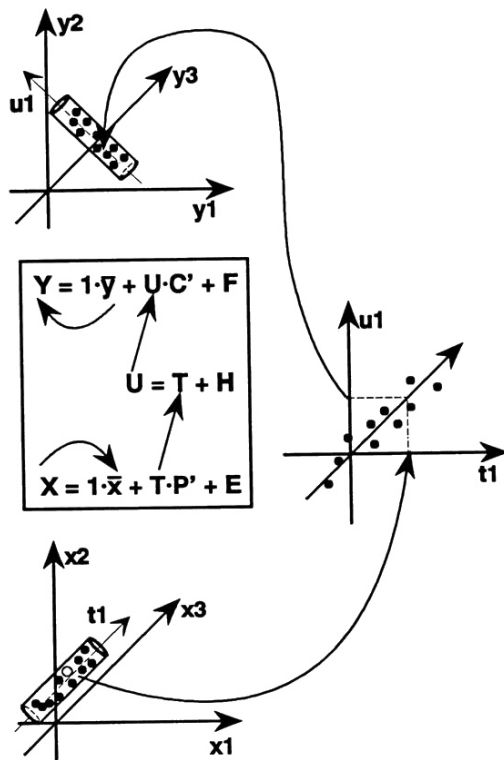


Figure 5. Geometrical presentation of the PLS method (Eriksson 1991).

### 3.3 Validation of models in PCA and PLS

The number of significant PCA or PLS components is usually determined using a method called cross-validation (CV). With CV the dataset is divided into  $X$  groups of typically 5-10 objects (Eriksson *et al* 1999). A model is fitted for the dataset with one group excluded. The excluded group is predicted by the model and the difference between the actual and the predicted value is calculated. In PCA, the objects are diagonally excluded while in PLS the objects are excluded in parallel rows. This process is repeated  $X$  times and then all partial predictions are summarised, providing a measure of the predictive power of the model, which can be expressed as the goodness of prediction ( $Q^2$ ) for each component. The goodness of fit is expressed by the  $R^2$  value.  $R^2$  and  $Q^2$  values range between 0-1. Ideally, the value of both should be large, and the difference between  $R^2$  and  $Q^2$  should not be too large, preferably not more than 0.2-0.3.

Especially in PLS modelling, external validation is preferred, i.e. prediction of an external set of data with known  $y$ -responses by the model, based

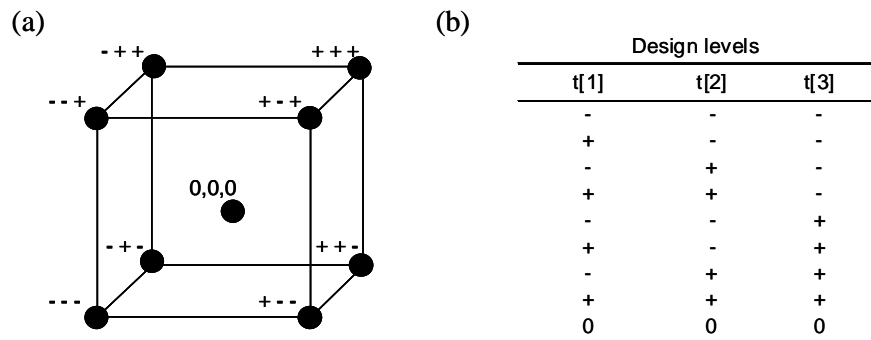
solely on the training set. The difference between the predicted and known  $y$  values will indicate the predictive power of the model. In Paper IV the initial intention was to do an external validation, but since there were too few accidents in the training set to construct a reliable model it was decided to use both the training and the validation sets as a single, combined set for the modelling.

### 3.4 Statistical design

During the selection of representative accidents (Paper II) the subset of chemical accidents needed to be selected in such a way that it would cover a sufficient range of variation in all the important variables for the index. By using statistical multivariate design approaches, such as factorial (FD) or fractional factorial designs (FFD), schemes are generated that introduce systematic variation of all variables simultaneously. Varying all the variables at the same time in such a systematic way will ensure that the whole experimental area is investigated, as described by Box *et al* (1978).

In the studies discussed in this thesis, the “experiments” were chemical accidents, which contained natural and uncontrolled data, and they could not be performed at the desired combination of variables and levels. In addition, the more or less correlated accident-describing variables (see Table 1, Section 2.2) needed to be condensed into a few dominant and orthogonal descriptors before a statistical design could be applied. By subjecting the data table to principal component analysis, new descriptors were derived. These new variables, the principal components (PC:s) which summarise the information present in the original variables, are also commonly referred to as principal properties (PP:s), as described by Skagerberg (1989). PP:s can be used as design variables because they are few in number, orthogonal and contain most of the information in the data from which they were derived. Hence, this method, *statistical multivariate design*, allows a large number of variables to be included in the design.

Mathematically, the selection was based on a two-level, full factorial design for the derived principal properties, i.e. the score values (Figure 6a and b). The design was complemented with three centerpoints to provide information about the possible curvature and to give rough estimates of quadratic and interaction terms. The selections were made according to a  $2 \cdot 2^3$  (= 16 accidents) design. This means that from each design level two representative accidents were selected.



**Figure 6.** Full factorial design (a) and the way the score vectors are used as principal properties in the design (b).

## 4 Initial evaluation of the EAI

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The initial evaluation of the EAI started in 1996 and the results of this evaluation are summarised below (for further description see Paper I and Scott 1997). More detailed descriptions of the EAI formula<sup>11</sup> and the variables are given in section 1.4. The initial evaluation of EAI was performed in two stages.

### 4.1 Stage I - test of EAI on chemical accidents

The purpose of Stage I (Paper I) was to evaluate the possibility of using the original EAI to classify the accidents into the risk categories (i.e. the classification scale) corresponding to the observed consequences. Table 2 presents the calculated EAI value for each of the 21 chemical accidents.

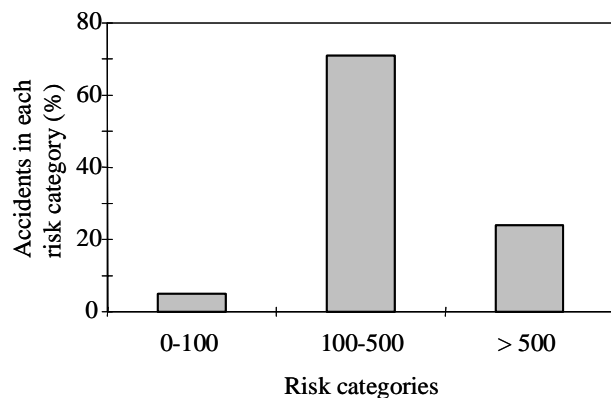
**Table 2.** Calculated EAI values for the 21 chemical accidents, together with the calculated values for the SP and the amount of chemical remaining in the ground or water environment.

| Accident no. | Place of accident: | Chemical involved:           | Type of accident:  | EAI values: | SP | Residual (%) |
|--------------|--------------------|------------------------------|--------------------|-------------|----|--------------|
| 1            | Kopparberg         | aluminium chloride (sol)     | transport accident | 432         | 18 | 74           |
| 2            | Bräcke             | gasoline                     | transport accident | 480         | 12 | 10           |
| 3            | Kristinehamn       | hydrochloric acid 38%        | transport accident | 320         | 16 | 15           |
| 4            | Karlshamn          | diesel fuel/heating oil no.1 | transport accident | 600         | 15 | 18           |
| 5            | Källered           | ferric chloride (sol)        | transport accident | 480         | 16 | 20           |
| 6            | Oxelösund          | benzene                      | industrial         | 1280        | 16 | 45           |
| 7            | Torshälla          | hydrofluoric acid            | industrial         | 340         | 17 | 21           |
| 8            | Kotka              | chlorobenzene                | oil harbour        | 960         | 12 | 46           |
| 9            | Solna I            | diesel fuel/heating oil no.1 | oil storage        | 240         | 10 | 5            |
| 10           | Solna II           | kerosene/jet fuel            | transport accident | 600         | 15 | 21           |
| 11           | Lycksele           | diesel fuel + gasoline       | transport accident | 480         | 12 | 26           |
| 12           | Norrhälje          | gasoline                     | transport accident | 480         | 12 | 8            |
| 13           | Ronneby            | sodium formate (sol)         | harbour            | 190         | 19 | 0.3          |
| 14           | Sundsvall          | phenol                       | industrial         | 504         | 9  | 2            |
| 15           | Hangö              | methyl methacrylate          | industrial         | 260         | 13 | 50           |
| 16           | Grängesberg        | gasoline                     | gas station        | 400         | 10 | 7            |
| 17           | Helsingborg        | diesel fuel/heating oil no.1 | transport accident | 480         | 12 | 4            |
| 18           | Åstorp             | methanol                     | transport accident | 60          | 12 | 6            |
| 19           | Norrhälje          | diesel fuel/heating oil no.1 | transport accident | 400         | 10 | 16           |
| 20           | Haninge            | kerosene/jet fuel            | transport accident | 400         | 10 | 8            |
| 21           | Robertsfors        | diesel fuel/heating oil no.1 | diesel storage     | 288         | 12 | 16           |

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<sup>11</sup> EAI = Am · Tox (Con + Sol + Sur)

The distribution (in percentages) of the calculated EAI values for the 21 accidents in the different risk categories is shown in Figure 7.

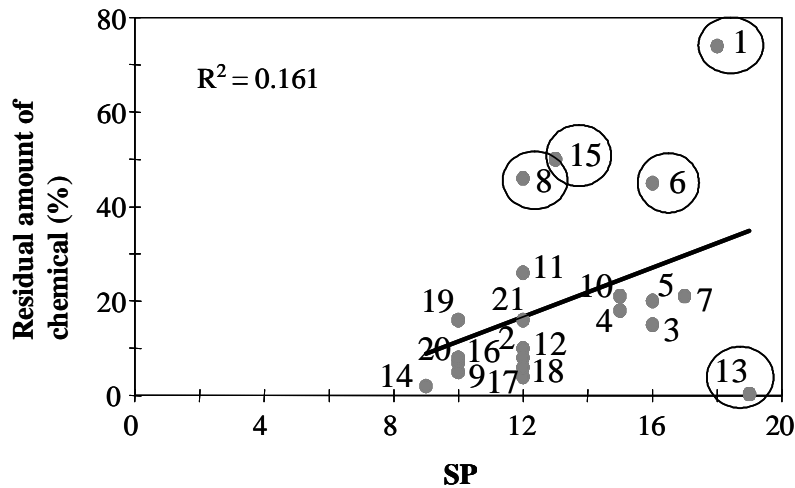


**Figure 7.** Distribution of the calculated EAI values in the risk categories (%).

The results showed that 71% of the accidents were classed in risk category 100-500 and only 5% in category 0-100. More than half of the material in this study (57%) consisted of transport accidents and accidents with petroleum products (52%). As the properties of the chemicals involved are the same in both of these types of accident, and the transported amounts were similar, their Tox, Con, Sol and Am values were similar and, hence, so were their EAI values. This finding also shows that the inherent chemical properties and the amount of chemical involved strongly influence the EAI value. Further, the calculated EAI values corresponded quite well to the observed consequences of the accidents, since accidents with no, or minor, consequences for the environment were placed in the lowest category while those with major consequences were placed in the highest risk category. However, there was a tendency for the index to overestimate the effects of some accidents with minor or unknown effects, and thus place these accidents in category 100-500.

The next step in Stage I was to calculate the amount of the released chemical remaining in the ground or water environment following the accidents (Table 2). This residual amount of chemical was then plotted versus the sum of the so-called Spreading Part (SP), i.e. the Con, Sol and Sur variables. This test was applied to investigate whether a higher value of the SP could have any correlation to the amount of chemical remaining in the ground or water environment (Figure 8). A reasonable assumption is that a higher value for the SP should lead to a larger amount of the chemical remaining in the ground or water environment.

Residual  
chemical in the environment (%) =  $\frac{\text{amount of chemical remaining after decontamination}}{\text{amount of chemical released}} \cdot 100$



**Figure 8.** Residual amount of chemical remaining in the ground or water environment versus SP.

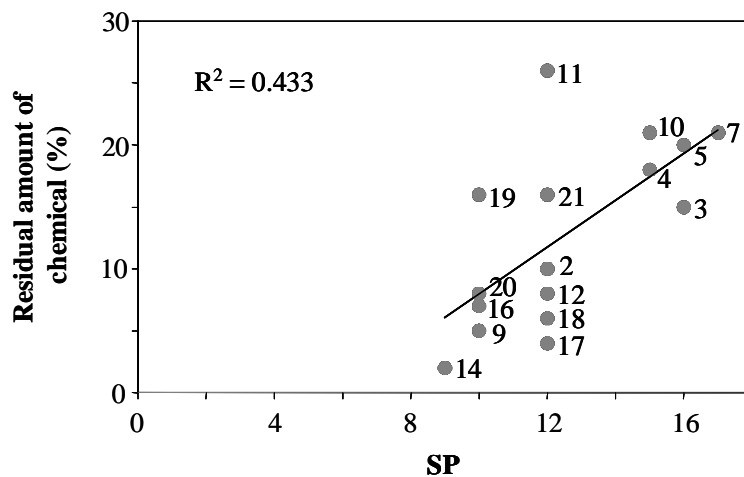
As shown in Figure 8, there was a weak linear correlation ( $R^2 = 0.161$ ) between SP and the residual chemical. However, large variations in all SP levels could be seen, implying that the SP did not have the capacity to predict the magnitude of the risk of a chemical spreading. In the plot, five outlying accidents can be identified (1, 6, 8, 13 and 15), which are described in more detail below.

- *Accident 1:* The discharged chemical reacted with water and the chemical was difficult to remove. Hence a large amount of chemical remained in the ground or water environment. The EAI does not include reactivity, and this accident can be regarded as an outlier.
- *Accident 6:* A large amount of a chemical with high volatility was discharged below ground level, and its spread was uncontrolled. A large amount of the chemical evaporated and the conditions made decontamination difficult. The high volatility and uncontrolled spread generated uncertainty in the amount of the chemical remaining in the environment.
- *Accident 8:* After this accident the decision was taken not to decontaminate the site affected by the released chemical completely because it settled (due to its density,  $1110 \text{ kg/m}^3$ ) into the ground

sediment, thereby complicating the decontamination process. Hence, a large amount, 46%, was left in the ground.

- *Accident 13*: The amount of the chemical remaining in the environment could not be reliably estimated because a large proportion of the supposedly removed amount probably consisted of rainwater. Hence, the true amount remaining was probably larger than the calculated value.
- *Accident 15*: After this accident it was decided not to decontaminate but to allow the chemical to evaporate. Since it is difficult to estimate the evaporated amount and the quantity of chemical that reached the ground or water environment, the remaining amount of chemical was uncertain.

As already mentioned in Chapter 1, many factors influence the spread of a chemical. For each of the outliers in Figure 8, the factors reactivity, volatility, weather and density appeared to influence the spread of the chemical, and hence the quantity that could be removed. The fact that the EAI only includes some of these factors (Con, Sol and Sur) limits its applicability. Figure 9 shows the fit of the model when accidents considered to be outliers were excluded.



**Figure 9.** Residual amount of chemical remaining in the ground or water environment versus SP, when the outliers were excluded.

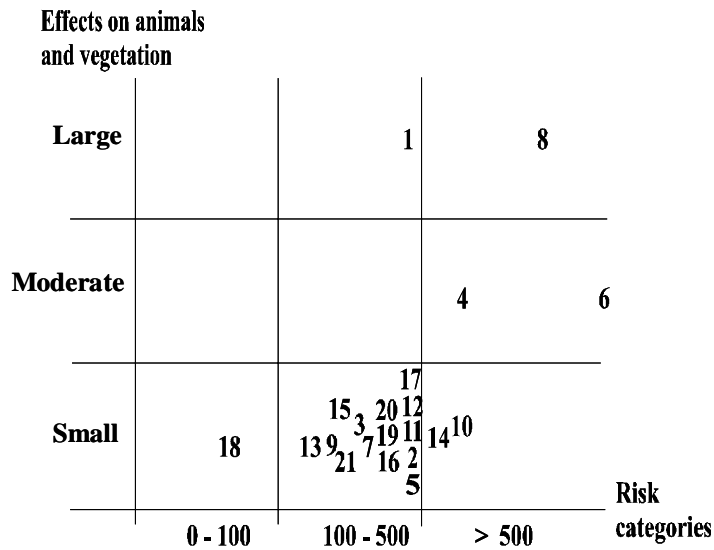
The results shown in Figure 9 implies that variables controlling the missing factors described above needed to be included in the EAI. Volatility and density were therefore added in the following steps of the EAI development

(Papers II -IV). Reactivity is a complex factor for which relevant descriptor variables are hard to identify. It was therefore decided that reactivity should not be included in the EAI. The weather, in turn, depends on the season, which is difficult to include in the EAI and instead is a factor that has to be judged from case to case as a complement to the EAI.

Another interesting fact that can be seen in Table 2 is that the calculated SP is a very minor part of the calculated EAI and that its variance is low. Hence SP has a weak influence on the calculated EAI, and because Sur in turn is a minor part of SP this variable has an even weaker influence on EAI.

In the subjective judgements of the 21 accidents the effects on organisms and vegetation, technical equipment and the length of the decontamination process of the 21 accidents were estimated (*Scott 1997; Scott 1998*). The purpose of these judgements (Figures 10-12) was to determine if a large effect in the environment will be correlated with a high EAI value, and vice versa, and to find out if the classification scale had to be changed. In the figures each accident corresponded to a number (Table 2). For an accident to be considered to have a correct position in the diagram, its effects had to be correlated to its EAI level, i.e. accidents with small effects should give an EAI of 0-100, while those with moderate and large effects should give EAI values of 100-500 and >500, respectively.

Effects on vegetation and animals were divided into small, moderate and large, and plotted together with the corresponding EAI values (Figure 10). A small effect could, for example, consist of local effects on trees, vegetation and microorganisms.



**Figure 10.** *Effects on vegetation and animals - calculated EAI values for 21 chemical accidents*

The data in Figure 10 show that effects on vegetation and animals in most cases were small, although a majority of the accidents obtained EAI values between 100-500. The effects of these accidents (2, 3, 5, 7, 9, 11, 12, 13, 15, 16, 17, 19, 20 and 21) appear to be overestimated by the EAI, as do those of accidents 10 and 14, which have EAI values greater than 500. The correctly positioned accidents were accidents 18, 8 and possibly 4. Notably, accident 1, which has large effects in the aquatic environment, only obtained an EAI value of 432.

Effects on technical equipment were divided into no effects, effects and large effects (Figure 11). A large effect could include, for example, the elimination of a wastewater treatment or water supply plant. According to Figure 11, ten accidents did not affect industrial equipment. Of these ten, eight (accidents 1, 2, 3, 5, 11, 12, 13 and 19) obtained EAI values between 100-500 and their effects appear to be overestimated by the EAI. There were seven accidents with EAI values between 100-500 (7, 9, 15, 16, 17, 20 and 21) together with accidents 18, 14 and 4 and possibly also accident 10 that were correctly positioned

| Effects on technical equipment |         | Risk categories |                |   |
|--------------------------------|---------|-----------------|----------------|---|
|                                | 0 - 100 | 100 - 500       | > 500          |   |
| Large effects                  |         |                 | 14 4           |   |
| Effects                        |         | 15 9<br>7 21    | 20 16<br>17 10 | 6 |
| No effects                     | 18      | 13 3<br>1 19    | 12 11<br>2 5   | 8 |

**Figure 11.** *Effects on industrial equipment - calculated EAI values for 21 chemical accidents*

The length of the decontamination process following the accidents was divided into classes of less than 1 month, 1-12 months and more than 12 months. As shown in Figure 12, most of the accidents had a decontamination time of 1-12 months. Of these accidents 1, 2, 3, 7, 12, 15, 16, 19, 20 and maybe 4, 10 and 14 were correctly estimated by the index. Only seven accidents had a decontamination time of less than a month, six of which (5, 9, 11, 13, 17 and 21) were overestimated by the index since they had EAI values between 100-500. In addition, accident 6, with a decontamination time of more than 12 months was also correctly estimated

| Time of decontamination | Risk categories |                                   |               |
|-------------------------|-----------------|-----------------------------------|---------------|
|                         | 0 - 100         | 100 - 500                         | > 500         |
| > 12 months             |                 |                                   | 6             |
| 1 - 12 months           |                 | 20<br>7 19 12<br>15 3 16 2 4<br>1 | 10<br>8       |
| < 1 months              | 18              | 13 <sup>9</sup> 21                | 17<br>11<br>5 |

**Figure 12.** Time of decontamination vs. calculated EAI for 21 chemical accidents

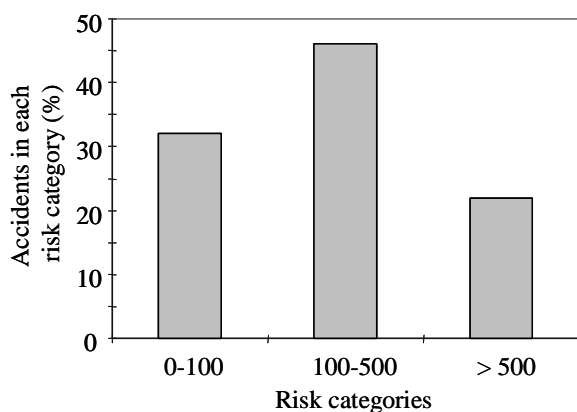
Overall, the subjective judgements demonstrated that there was a correlation between the effects and the calculated EAI values. Although some accidents were not correctly estimated by the index, most of them were. The main conclusions from the results plotted in Figures 10-12 were that the proposed risk categories functioned quite well and that the classification scale did not need to be changed.

#### 4.2 Stage II - theoretical test

The theoretical sensitivity test (*Scott 1997; Scott 1998*) was designed to analyse how the variables in the formula influence the magnitude of the EAI, and to find out if the resulting EAI values were spread usefully across all three risk categories. The test was performed in such a way that one variable at a time was varied while the other variables in the formula were given a fixed value (see Appendix II for calculations).

In summary, the results of these calculations showed that the variables related to the spread of the chemical (Con, Sol and Sur) had less influence on the magnitude of the index than the amount (Am) and toxicity (Tox). Secondly, the variables Am and Sur were varied and EAI was calculated for 49 different chemicals. Since the parameters Sur and Am can be varied independently, thereby creating 25 different “accident situations”,  $49 \cdot 25 = 1225$  permutations were generated (see Appendix III for an example). Indices were calculated for all of these permutations, to examine the

distribution of the EAI values into the three different risk categories, and to see how well the classification scale worked. The results, presented in Figure 13, showed that the distribution is relatively even. Of the 1225 EAI values calculated in this test, the highest frequency (46%) was in risk category 100-500, while 32% and 22%, respectively, were in the two other categories. The results showed no extreme predominance of any risk category, but rather an even distribution, so no change in the ranges of the classification scale seemed necessary.



**Figure 13.** Distribution (%) of the calculated EAI values in the three risk categories

The conclusions reached in Paper I and the Swedish report (*Scott 1997*) were as follows:

- EAI has the capacity, with a few modifications, to be a useful tool for ranking and classifying the environmental consequences of chemical accidents. Thus, it could be used to evaluate what further risk assessment (if any) should be performed.
- Since there was insufficient information and documentation about some of the chemical accidents, only 21 accidents were available for the study, most of which were transport accidents. Transport accidents are often similar since the amount transported is limited, and the transported chemical is a petroleum product in approximately 80% of such cases. This may lead to bias in the representativity of the EAI. Therefore it was necessary to collect a more extensive accident database and to develop a strategy for selecting representative material. These steps are presented in Paper II and Chapter 5.

- The results of the evaluation suggested that the variable Sur should be strengthened and that a volatility variable should be added to the index. In particular, it was shown during the calculations of SP and the theoretical sensitivity test that the variable Sur has a very low impact on the magnitude of the EAI. The changes to be made should therefore strengthen the variable Sur, and perhaps add a variable to EAI expressing volatility.

Based on these conclusions the following changes were made:

- A variable describing the volatility ( $P_v$ ) was included. To strengthen the variable Sur, the type of soil was replaced by two new parameters (hydraulic conductivity,  $K'$  and porosity,  $n$ ). A variable regarding the density,  $D$ , was also included as it helps to describe the vertical transport of a chemical.
- Following the introduction of the new variables the EAI formula has to be changed and reorganised, perhaps as follows:

$$EAI_2 = EAI_1 + k_1(\text{new variable}) + k_2(\text{new variable}) \dots k_n(\text{new variable})$$

The constants  $k_1, k_2 \dots k_n$  in the formula represent the weight of the variables.

## 5 Selection of a representative set of chemical accidents

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The first valuation of the EAI showed that more extensive and diverse accident material was needed. Subsequently, data on 42 additional chemical accidents were assembled and included in the dataset. This new dataset had an overrepresentation of accidents with petroleum products (69%), and was thus skewed with respect to chemical properties. To address the above problems a method was needed to select a representative subset of accidents to work with in the model development process (Paper II). The subset of accidents to be used in the development of the index had to be selected in an unbiased way. The selection should:

- include good representatives of the chemical accident domain with respect to both chemical properties and site-specific properties, and
- efficiently span the domain

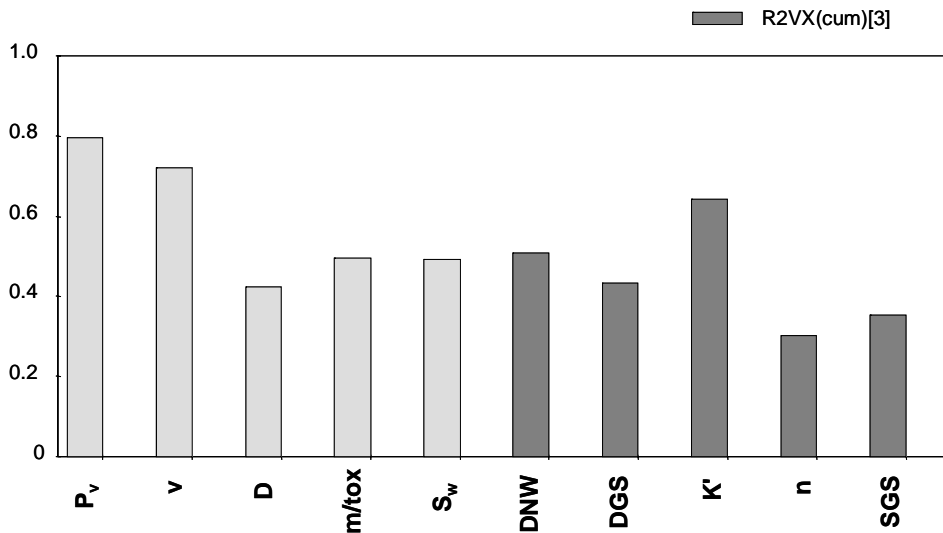
As the chemical property variables are correlated, PCA and statistical multivariate design were used in the selection procedure because this method can handle correlated data. A more detailed description of multivariate methods and statistical design is given in Chapter 3.

### 5.1 Selection procedure

The dataset consisted of 55 chemical accidents (objects), since three accidents were excluded, each of which was described by 10 variables: chemical property variables ( $v$ ,  $D$ ,  $S_w$ ,  $P_v$  and  $Tox$ ), the amount ( $m$ ), and site-specific properties ( $DGS$ ,  $DNW$ ,  $SGS$ ,  $K'$  and  $n$ ). Additional information about the accidents and property variables is given in Chapter 2, Table 1, and detailed information about the models is found in Paper II.

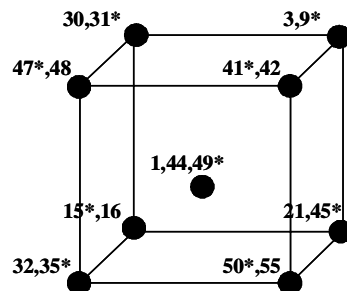
Using PCA a three-dimensional model was developed for the whole data set. The model explained 51% ( $t[1]:22,3\% + t[2]:16,7\% + t[3]:12,5\%$ ) of the variation and showed that score vector 1 ( $t[1]$ ) was explained mainly by chemical property variables and, hence, the chemical property vector. Site-specific properties influenced mainly  $t[2]$  and  $t[3]$ , which are therefore site-specific property vectors. The principal components were then used as new variables for a statistically representative selection as they summarise the major information present in the original variables. In the score plot of the PCA, chemical accidents that were well separated from each other were obvious candidates for selection, because they represent a systematic spread

in all properties. The model overview, Figure 14, shows that site-specific properties (dark-grey) and the inherent chemical properties (light-grey) are approximately equally important for the model.

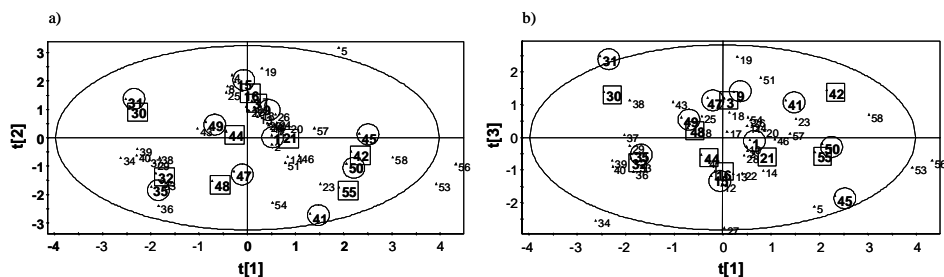


**Figure 14.** Model overview. Shows the extent to which each contributes to the model according to three calculated components. From 0 = no contribution to 1 = total contribution. The site specific properties and the chemical properties are coloured dark-grey and light-grey respectively.

When the calculated total score vectors (t[1]-t[3]) were used as design variables in a  $2^3$  full factorial design (see Chapter 3.4), 5-10 chemical accidents were found at each of the eight design levels. Figure 15a shows the selected training and validation sets based on this design and 15b the new labels of the accidents in each set. In Figure 16a the selected accidents are marked in the score plots.



**Figure 15.** A  $2^3$  design with the selected chemical accidents at each design level. Accidents that form the training set (TS) are marked with \* and the unmarked accidents belong to the validation set (VS).

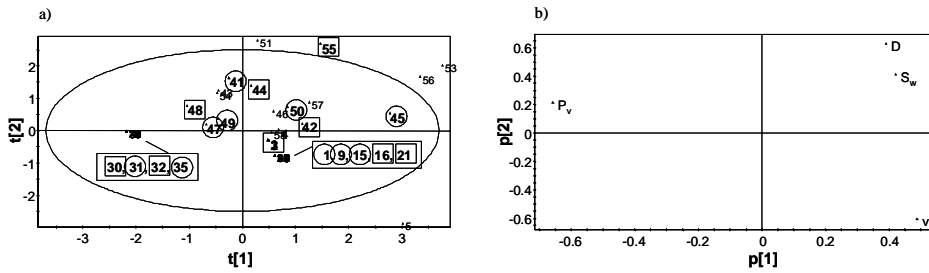


**Figure 16.** Selected training and validation set in a) the score plot of the two first components,  $t[2]/t[1]$  and b) the first and the third components,  $t[3]/t[1]$ . Accidents in the training set are marked with a circle, and accidents in the validation set are marked with a square.

Since both a training and a validation set were selected, the design was applied twice ( $2 \cdot 2^3 = 16$  accidents), which means that two representative accidents were selected from each design level, together with, in total, three centre-points. This generated eight accidents in each set, complemented with two and one centre-points respectively. During the selection, the most extreme accidents were avoided and other knowledge about the accidents (such as the magnitude of available information, investigations made after the accident etc) was also considered.

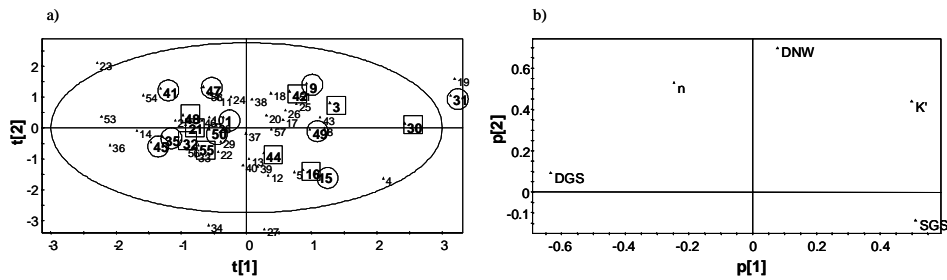
## 5.2 Results of the selection

Depending on in which of the quadrants the chemical accidents are positioned they will represent different spreading scenarios with respect to chemical inherent properties (Figure 7). The selected accidents did not cover all quadrants, and hence not all types of spreading scenarios. However, since the original dataset based on real cases did not have balanced coverage of all four quadrants either, the selected accidents could be regarded as the best possible covering the actual situations.



**Figure 17.** Plot illustrating the coverage of the range of variation in chemical properties for the selected accidents, a) variable scores,  $t[2]/t[1]$ , and b) variable loadings,  $p[2]/p[1]$ . Hotelling's  $T^2$  (0.05) is given by the tolerance ellipse.

Of the site-specific variables only the porosity of the soil,  $n$ , is less well explained as seen in Figure 18b. The four quadrants will represent different spreading scenarios, based on the positions of the variables. The score plot (Figure 18a) shows that the selected accidents represent the different spreading scenarios well, and will be good representatives of the original dataset with respect to site-specific properties.



**Figure 18.** Plots illustrating the coverage of the range of variation in site-specific properties for the selected accidents] a) variable scores,  $t[2]/t[1]$ , and b) variable loadings,  $p[2]/p[1]$ . Hotelling's  $T^2$  (0.05) is given by the tolerance ellipse.

To see if all possible accident scenarios in the whole dataset, as described by the chemical and site-specific variable span, are represented by the selected accidents, each variable span was investigated. For example: variable  $n$  ranges between 0 and 55 in the whole dataset and this span is also represented by the accidents in the selected set, as seen in Table 3 (also shown by Figure 6 in Paper II).

The results presented in Table 3 show that all variables appear to be quite well represented, within their respective ranges, in the selected training and validation set except for  $SGS$  and  $DNW$ .  $SGS$  has one and  $DNW$  two

accident scenarios missing. *SGS* lacks the class 0.1; no well lake or watercourse in the area, but this is a low-risk scenario and it will probably not cause any underestimation of the situation when using the EAI in the future. *DNW* lacks the scenario  $DNW=0.01$ ; release of chemical directly into water. This scenario could be underestimated. However, other accidents with a *DNW* of 2-5 m (accidents 32, 35, 45, 21 and 15 in Figure18) can be regarded, more or less, as spills into water since the distance to the watercourse in each these cases was very short and therefore cover for the lacking scenario. *DNW* also lack scenarios where the chemical spill occurred a very long distance from a watercourse (2000 m in the whole dataset compared to 300 m in the selected dataset). However, 2000 m distance from a watercourse is regarded as a low risk scenario, implying that the EAI will not underestimate the situation when using it.

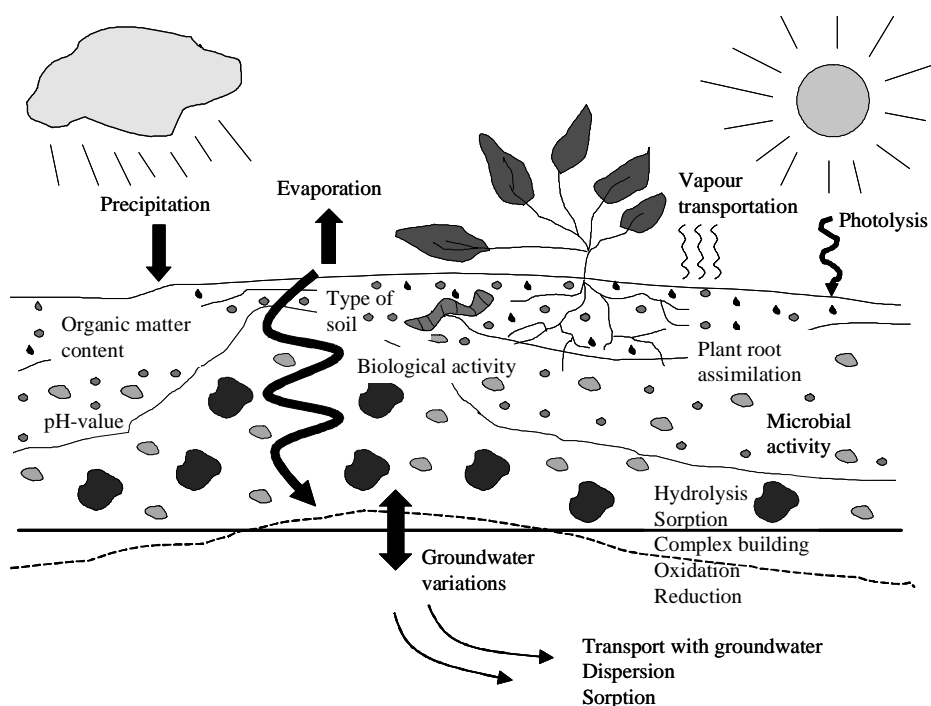
**Table 3.** The table shows the span of each variable for the whole dataset and for the selected dataset

| Variables | Span of whole dataset | Span of selected dataset |
|-----------|-----------------------|--------------------------|
| $P_v$     | 0 - 70                | 0 - 70                   |
| v         | 0.8 - 9.5             | 0.8 - 3.2                |
| D         | 750 - 1460            | 750 - 1370               |
| m/Tox     | 79000 - 1.6E+12       | 79000 - 2.1E+11          |
| $S_w$     | 0.001 - 90            | 0.001 - 90               |
| DNW       | 0.01 - 2000           | 2 - 300                  |
| DGS       | 0.01 - 33             | 0.01 - 33                |
| K'        | 0-3                   | 0 - 3                    |
| n         | 0 - 55                | 0 - 55                   |
| SGS       | 0.1 - 1               | 0.5 - 1                  |

In summary, the results from Paper II show that PCA and statistical multivariate design could be used to make an unbiased selection of a representative dataset for modelling and evaluation of the EAI. Further, evaluation of the selection demonstrated that both the descriptors for inherent chemical properties and properties of the surroundings were well described in the selected subset of chemical accidents. The only exceptions were the variables *SGS* and *DNW*, but the non-covered scenarios were either low-risk scenario or covered by other selected accidents. The selected subset of chemical accidents could thus be used to develop criteria to judge the environmental consequences of a chemical accident.

## 6 Estimating environmental effects using expert judgements

The environment is influenced by a variety of complex, interacting processes and at present no means have been developed for assessing effects to the whole system. Figure 19 shows some of the processes affecting the soil environment to illustrate this complexity.



**Figure 19.** Some of the diverse processes affecting the soil environment (after Kemakta Konsult AB 1996)

When developing an EAI model, estimates of the environmental effects (response values) are needed, but are not always easily accessible. Responses such as toxicity, degradation rate or bioaccumulation have been used previously, for example by Bello *et al* 1997 (see Section 1.3.2), but these responses apply solely to the specific chemical examined, and its test values obtained in a laboratory environment. Such measurements will, therefore, be poor estimates of the environmental effects caused by the chemical, so new methods must be generated. Questionnaires are commonly used in social sciences (Robinson 1998), but not regularly in natural science. The objective of the study reported in Paper III was to evaluate whether questionnaires and expert judgements could be used to collect useful data on the environmental consequences of chemical accidents. Based on the above

considerations, the method used for data collection was a questionnaire designed for assessing the environmental consequences of chemical accidents. The sampling unit for the questionnaires consisted of environmental health officers selected from a representative set of municipalities in Sweden (see Section 2.4 for a fuller description).

Table 4 describes the data set used in the study, consisting of two subsets (a training set, TS, and a validation set, VS), both of nine accidents. For further description of the accidents see Chapters 2 and 5. The 18 environmental health officers in the expert panel were divided into two groups, the larger of which (10 experts) judged the accidents in the TS, while the smaller group (seven experts) judged the VS set. The experts were given the questionnaires together with short summaries on each accident.

**Table 4.** Chemical accidents in the training and validation sets, together with their new accident numbers and some descriptors.

|                | <i>Accident number in dataset</i> | <i>Number in this study</i> | <i>Chemical:</i>           | <i>CAS-no:</i> | <i>m (metric tonnes)</i> | <i>Tox (mg/l)</i> | <i>DNW (m)</i> | <i>DGS (m)</i> |
|----------------|-----------------------------------|-----------------------------|----------------------------|----------------|--------------------------|-------------------|----------------|----------------|
| Training set   | 9                                 | 1                           | Dieselfuel/heating oil No1 | 68334-30-5     | 24.6                     | 2.6               | 100            | 5.0            |
|                | 15                                | 2                           | Dieselfuel/heating oil No1 | 68334-30-5     | 24.6                     | 2.6               | 5              | 0.2            |
|                | 31                                | 3                           | Gasoline                   | 86290-81-5     | 38.2                     | 4.9               | 100            | 0.01           |
|                | 35                                | 4                           | Gasoline                   | 86290-81-5     | 35.5                     | 4.9               | 2              | 1.87           |
|                | 41                                | 5                           | Methanol                   | 67-56-1        | 35                       | 13200             | 125            | 33.0           |
|                | 45                                | 6                           | Phenol                     | 108-95-2       | 90                       | 3.3               | 4              | 4.1            |
|                | 47                                | 7                           | n-Butylacetate             | 123-86-4       | 4.8                      | 18                | 25             | 23.0           |
|                | 49                                | 8                           | Styrene                    | 100-42-5       | 60                       | 9.1               | 1              | 3.1            |
|                | 50                                | 9                           | 4-Chloro-m-cresol          | 59-50-7        | 0.002                    | 7.6               | 200            | 1.5            |
| Validation set | 3                                 | 1                           | Kerosene/Jet fuel          | 8008-20-6      | 24.2                     | 3.1               | 15             | 1.5            |
|                | 16                                | 2                           | Dieselfuel/heating oil No1 | 68334-30-5     | 37                       | 2.6               | 7              | 0.35           |
|                | 21                                | 3                           | Dieselfuel/heating oil No1 | 68334-30-5     | 13.1                     | 2.6               | 5              | 8.0            |
|                | 30                                | 4                           | Gasoline                   | 86290-81-5     | 28.5                     | 4.9               | 25             | 0.01           |
|                | 32                                | 5                           | Gasoline                   | 86290-81-5     | 35.3                     | 4.9               | 2              | 16.0           |
|                | 42                                | 6                           | Iso-propanol               | 67-63-0        | 0.18                     | 2285              | 300            | 2.0            |
|                | 44                                | 7                           | Chlorobenzene              | 108-90-7       | 1000                     | 4.7               | 30             | 2.3            |
|                | 48                                | 8                           | Vinylacetate               | 108-05-4       | 29.8                     | 18                | 7              | 7.6            |
|                | 55                                | 9                           | Formic acid                | 64-18-6        | 6.1                      | 70                | 30             | 3.2            |

The questionnaires consisted of two parts. Part I concerned the background of the experts (see Paper III) and Part II concerned their judgements. Each question in the latter section was related to an environmental effect (response).

The experts judged both the short-and long- term effects of each accident on:

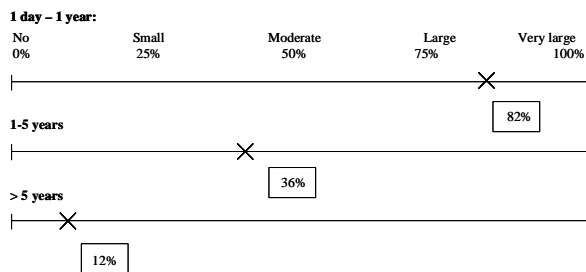
- 1A. Animal life in the aquatic environment
- 1B. Ground-living animals and microorganisms
- 1C. Animals in the terrestrial (above ground) environment
- 2A. Vegetation in the aquatic environment
- 2B. Vegetation in the terrestrial environment
- 3A. The potential for using groundwater and surface water fo drinking water
- 3B. The potential for using land and water for economic activities, such as growing crops, forestry, commercial fishing and building
4. Vital installations such as wells, cables, sewage systems, and water treatment plants etc
5. The potential of the site for outdoor life and recreational pursuits such as fishing (angling), walking, trekking and swimming

Questions 1A, 1B and 1C are related to effects on animal life. Questions 2A and 2B cover effects on vegetation. Questions 3A, 3B and 5 are related to effects on the use of the environment for different activities. Question 4 differs from the other questions as it solely concerns effects on man-made installations.

The experts made their judgements for each response on a continuous scale varying from 0% to 100% effect for three different periods of time: 0-1 years, 1 – 5 years, and > 5 years after the accident. An example of a question can be seen in Table 5.

**Table 5.** Example of a question. Judgement of effects on animal life in the aquatic environment of an accident in the training set.

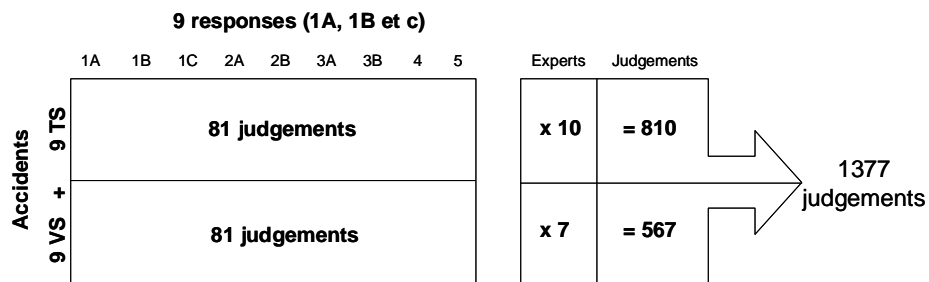
*1a.* How do you judge the effects on **animal life** in the aquatic environment, within the accident area, in a short and long term perspective?



### 6.1 Results of the judgements

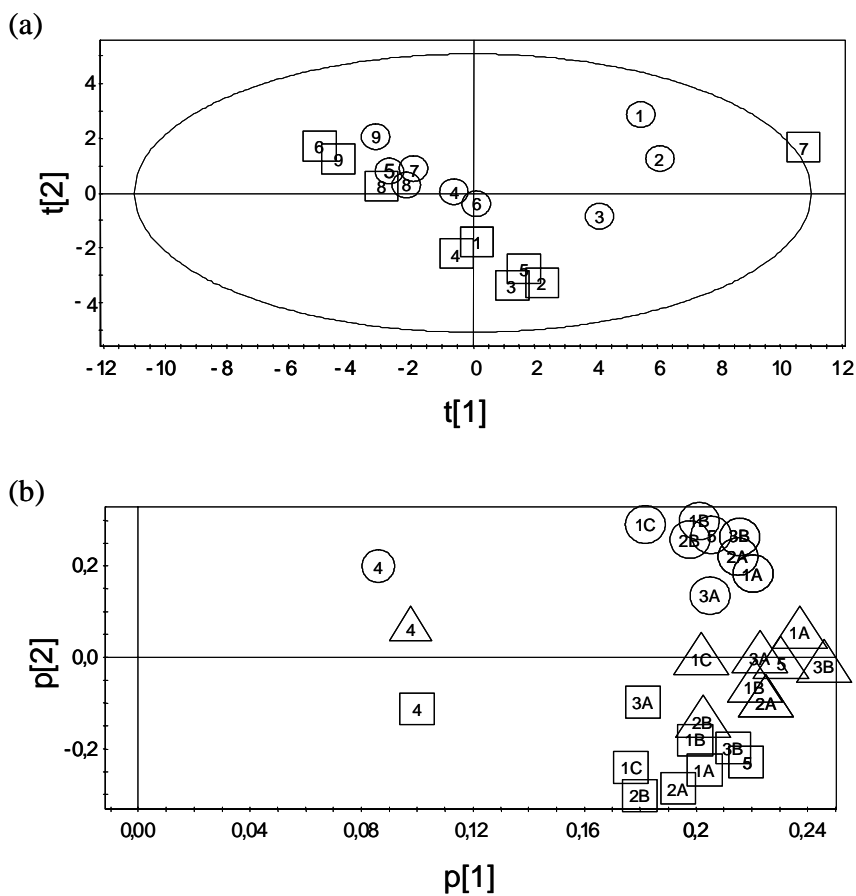
The results from part I of the questionnaire showed that the two groups of experts were comparable with respect to all characteristics except education. Twice as many experts in the training set as in the validation set were formally educated as environmental officers. In contrast, three of the experts in the validation set, but only one in the training set, had a similar, but older, type of education in the environmental field. However, the results did not indicate that differences in education between the two sets were associated with any significant differences in their judgements.

The judgements resulted in a data matrix consisting of a TS with 810 judgements, and a VS with 567 judgements. Figure 20 illustrates the dimensions of the data matrix.



**Figure 20.** The extent of the data matrix.

To overview all judgements as described by the median estimated effect for each question (response) and accident in the TS and VS a five component PCA model was developed, which explained 91.8% of the variance. Figure 21 shows (a) the variable scores and (b) the variable loadings of the two first components in the model.



**Figure 21.** Chemical accidents described by the medians of the judged response values. (a) variable scores  $t[2]/t[1]$  for the accidents. Accidents in the TS are marked with circles and accidents in the VS are marked with squares; (b) variable loadings  $p[2]/p[1]$  for the responses (see Section 3.2). Responses for years 0-1, 1-5 and >5 are marked with squares, triangles and circles, respectively.

In the loading plot, showing the judgement of each response (Figure 21b), there is a clear division into three groups: short term (0-1 years), medium-term (1-5 years), and long-term (> 5 years) effects. The way each response influences the model can also be seen. Response variables far away from the origin of the plot are the most important, and those close to it are the least important.

The most important responses for the PCA model examining the judgements of the short-term perspective are 1A, 2A, 2B, 3B and 5. For years 1-5 responses 1A, 2A, 3B and 5 are the most important, and for > 5 years responses 1A, 1B, 2A, 3B and 5 are the most significant. Responses 1C and

3A (in the short-term perspective) have less influence on the model. On the other hand, variable 4 (effects on vital installations) appear to have little or no influence on the model. This is most likely an effect of the small variation in the judgements related to this response (the majority of the experts judged almost all the accidents as having no effect (0%) on such installation in the long-term) together with the fact that variable 4 is quite different in nature from the other variables.

The score plot in Figure 21a shows the chemical accidents in the training and validation sets. The accidents in the two sets show a similar distribution, apart from accident 7 in the validation set and accidents 1 and 2 in the training set, which diverge from the others. The reason for this divergence is that these accidents were judged to cause larger effects in a long-term perspective than the other accidents. Further, in Figure 21a, the accidents in the two sets are separated along  $t[1]$  according to their severity. Accidents 6 and 9 in the VS and 9 in the TS were judged to cause small environmental effects, while accidents 2, 3, and 5 in the VS and accident 3 in the TS, were judged to cause larger effects. A general pattern shown in Figure 21 is for the accidents in the two sets to be separated over both time and effect levels.

Table 6 shows the judgements of the effects (in %) of the accidents in the training set on (a) animal life in the aquatic environment (1A) and (b) the potential for using land and water resources (3B). Similarly, Table 7 shows the judgements of the accidents in the validation set for the same two responses. The other results from the judgements in the two sets are given in an appendix to Paper III. The different effect levels are colour-coded in the tables, with green, yellow, orange and red corresponding to Effect Levels (ELs) 0-25%, 26-50%, 51-75% and 76-100%, respectively.

As shown in Table 6, there are several clear trends in the training-set judgements. Generally, the experts on the panel agreed that the largest environmental effects occurred within 0-1 year of the accidents, and that the effects became smaller with time. This gives a rough indication of how long such accidents will affect the environment, and the scale of the effects, despite differences amongst the judgements on the relative strength of the effects. For example, the data on accident 2 in Table 6a, show that expert *a* judged the effects on animal life as follows: 93% (0-1 years), 71% (1-5 years) and 48% (>5 years) while the corresponding figures for expert *j* were 73%, 30% and 7%, respectively. This example shows that both experts agree that the effect will decline after 1-5 years and >5 years, but they differ in terms of the strength of the effects. Further, accidents 1 (in which diesel fuel was spilled close to a water catchment area), 2 (diesel fuel within a

water catchment area) and possibly also accident 3 (gasoline within a Natura 2000<sup>12</sup> area, containing a sensitive moss) in the training set were judged to cause larger effects in comparison to the others, especially after > 5 years (Table 6a and 6b).

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<sup>12</sup> Natura 2000 is the EU network for protected types of nature and species.

**Table 6.** The judgements regarding effects of the accidents (in %) in the training set on (a) animal life in the aquatic environment (response 1A) and (b) the potential for using land and water resources (response 3B). Judgements by the experts in the training set are marked with the letters a-j in the table.

a)

| Accidents: | 0-1 year |    |     |    |    |     |    |    |     |    | 1-5 years |    |    |    |    |    |    |    |    |    | > 5 years |    |    |    |    |    |    |    |    |    |
|------------|----------|----|-----|----|----|-----|----|----|-----|----|-----------|----|----|----|----|----|----|----|----|----|-----------|----|----|----|----|----|----|----|----|----|
|            | a        | b  | c   | d  | e  | f   | g  | h  | i   | j  | a         | b  | c  | d  | e  | f  | g  | h  | i  | j  | a         | b  | c  | d  | e  | f  | g  | h  | i  | j  |
| 1          | 93       | 73 | 75  | 70 | 84 | 75  | 62 | 84 | 100 | 50 | 50        | 49 | 50 | 70 | 66 | 50 | 24 | 51 | 75 | 34 | 37        | 49 | 25 | 25 | 35 | 25 | 0  | 24 | 75 | 9  |
| 2          | 93       | 82 | -   | 85 | 82 | 75  | 96 | 96 | 100 | 73 | 71        | 36 | -  | 85 | 63 | 75 | 74 | 48 | 75 | 30 | 48        | 49 | 12 | -  | 49 | 50 | 24 | 48 | 75 | 7  |
| 3          | 96       | 82 | 100 | 85 | 72 | 100 | 95 | 72 | 100 | 74 | 34        | 32 | 75 | 69 | 16 | 50 | 37 | 72 | 75 | 64 | 12        | 63 | 11 | 25 | 14 | 25 | 7  | 47 | 25 | 36 |
| 4          | 97       | 76 | 75  | 64 | 75 | 50  | 95 | 72 | 75  | 24 | 14        | 34 | 25 | 45 | 39 | 25 | 23 | 2  | 25 | 5  | 2         | 47 | 11 | 25 | 5  | 0  | 1  | 3  | 0  | 6  |
| 5          | 97       | 49 | 75  | 70 | 91 | 25  | 60 | 49 | 50  | 23 | 3         | 13 | 25 | 36 | 16 | 25 | 10 | 3  | 25 | 5  | 2         | 19 | 6  | 25 | 7  | 0  | 1  | 1  | 0  | 1  |
| 6          | 96       | 84 | 75  | 82 | 48 | 100 | 97 | 63 | 75  | 91 | 5         | 49 | 50 | 70 | 3  | 50 | 24 | 1  | 0  | 70 | 4         | 46 | 14 | 25 | 4  | 25 | 3  | 1  | 0  | 42 |
| 7          | 3        | 26 | 75  | 51 | 59 | 25  | 96 | 3  | 50  | 29 | 4         | 15 | 75 | 52 | 26 | 25 | 24 | 3  | 25 | 5  | 3         | 32 | 7  | 50 | 9  | 0  | 3  | 3  | 0  | 6  |
| 8          | 96       | 84 | 50  | 69 | 49 | 25  | 83 | 82 | 50  | 44 | 61        | 35 | 25 | 36 | 3  | 25 | 24 | 46 | 25 | 1  | 46        | 17 | 11 | 25 | 3  | 0  | 3  | 30 | 0  | 1  |
| 9          | 5        | 25 | 25  | 51 | 7  | 25  | 24 | 1  | 0   | 29 | 5         | 12 | 0  | 49 | 5  | 25 | 3  | 2  | 0  | 3  | 5         | 26 | 12 | 0  | 6  | 0  | 2  | 1  | 0  | 3  |

b)

| Accidents: | 0-1 year |    |     |    |    |     |    |    |     |    | 1-5 years |    |    |    |    |    |    |    |    |    | > 5 years |    |    |    |    |    |   |    |    |    |
|------------|----------|----|-----|----|----|-----|----|----|-----|----|-----------|----|----|----|----|----|----|----|----|----|-----------|----|----|----|----|----|---|----|----|----|
|            | a        | b  | c   | d  | e  | f   | g  | h  | i   | j  | a         | b  | c  | d  | e  | f  | g  | h  | i  | j  | a         | b  | c  | d  | e  | f  | g | h  | i  | j  |
| 1          | 96       | 61 | 25  | 48 | -  | 100 | 48 | 73 | -   | 36 | 24        | 50 | 25 | 48 | -  | 75 | 23 | 73 | -  | 24 | 25        | 23 | 25 | 48 | -  | 75 | 9 | 50 | -  | 3  |
| 2          | 96       | 49 | 100 | 89 | 95 | 75  | 96 | 64 | 100 | 46 | 35        | 18 | 50 | 94 | 49 | 50 | 32 | 49 | 50 | 28 | 25        | 6  | 25 | 67 | 12 | 25 | 3 | 43 | 25 | 4  |
| 3          | 96       | 72 | 100 | 18 | 1  | 100 | 49 | 78 | 75  | 70 | 49        | 13 | 75 | 21 | 1  | 50 | 14 | 60 | 25 | 55 | 7         | 7  | 50 | 21 | 1  | 25 | 3 | 24 | 0  | 14 |
| 4          | 3        | 35 | 75  | 62 | 61 | 50  | 24 | 49 | 75  | 7  | 3         | 11 | 50 | 62 | 9  | 50 | 2  | 14 | 50 | 2  | 4         | 7  | 25 | 30 | 6  | 25 | 2 | 12 | 25 | 2  |
| 5          | 95       | 25 | 75  | 68 | 11 | 25  | 64 | 1  | 25  | 26 | 3         | 2  | 25 | 45 | 18 | 25 | 11 | 1  | 0  | 9  | 1         | 3  | 25 | 12 | 4  | 0  | 3 | 0  | 0  | 4  |
| 6          | 97       | 74 | 75  | 74 | 63 | 100 | 49 | 49 | 75  | 71 | 5         | 32 | 25 | 76 | 4  | 25 | 3  | 23 | 25 | 48 | 4         | 7  | 25 | 67 | 3  | 0  | 3 | 23 | 0  | 26 |
| 7          | 3        | 24 | 75  | 80 | 91 | 25  | 25 | 50 | 25  | 6  | 4         | 9  | 75 | 78 | 51 | 25 | 4  | 3  | 0  | 7  | 3         | 7  | 50 | 53 | 22 | 0  | 4 | 3  | 0  | 7  |
| 8          | 96       | 25 | 50  | 50 | 83 | 25  | 24 | 0  | 0   | 25 | 48        | 9  | 25 | 46 | 5  | 25 | 4  | 0  | 0  | 2  | 7         | 5  | 25 | 30 | 6  | 25 | 4 | 0  | 0  | 2  |
| 9          | 97       | 12 | 25  | 25 | 66 | 0   | 12 | 24 | 1   | 25 | 51        | 5  | 25 | 43 | 0  | 12 | 2  | 1  | 0  | 2  | 52        | 5  | 25 | 28 | 0  | 0  | 3 | 1  | 0  | 1  |

**Table 7.** The judgements regarding effects (in %) of the accidents in the validation set on (a) animal life in the aquatic environment (response 1A) and (b) the potential for using land and water resources (response 3B). Judgements by the experts in the validation set are marked with the letters k-q in the table.

a)

| Accidents: | 0-1 year |     |     |    |     |     |     | 1-5 years |    |    |    |    |     |     | > 5 years |   |    |    |   |    |     |    |   |   |   |   |   |   |   |   |   |
|------------|----------|-----|-----|----|-----|-----|-----|-----------|----|----|----|----|-----|-----|-----------|---|----|----|---|----|-----|----|---|---|---|---|---|---|---|---|---|
|            | k        | l   | m   | n  | o   | p   | q   | k         | l  | m  | n  | o  | p   | q   | k         | l | m  | n  | o | p  | q   |    |   |   |   |   |   |   |   |   |   |
| 1          | 75       | 75  | 75  | 39 | 75  | 50  | 75  | 50        | 0  | 25 | 1  | 50 | 25  | 50  | 25        | 0 | 0  | 1  | 0 | 0  | 0   | 0  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |   |
| 2          | 75       | 100 | 100 | 97 | 75  | 50  | 75  | 25        | 50 | 50 | 24 | 25 | 25  | 50  | 25        | 0 | 0  | 2  | 0 | 0  | 0   | 25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3          | 75       | 100 | 100 | 0  | 100 | 75  | 75  | 25        | 0  | 25 | 1  | 50 | 25  | 50  | 25        | 0 | 0  | 1  | 0 | 0  | 0   | 25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4          | 75       | 100 | 50  | 97 | 75  | 75  | 75  | 50        | 25 | 25 | 16 | 0  | 25  | 25  | 25        | 0 | 0  | 1  | 0 | 0  | 0   | 0  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5          | 100      | 100 | 75  | 97 | 75  | 100 | 75  | 50        | 25 | 50 | 24 | 25 | 50  | 25  | 0         | 0 | 3  | 0  | 0 | 0  | 25  | 0  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6          | 25       | 25  | 50  | 1  | 25  | 25  | 50  | 0         | 0  | 25 | 1  | 0  | 0   | 0   | 0         | 0 | 0  | 1  | 0 | 0  | 0   | 0  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7          | 100      | 100 | 100 | 97 | 100 | 100 | 100 | 75        | 25 | 75 | 96 | 50 | 100 | 100 | 75        | 0 | 50 | 97 | 0 | 75 | 100 | 0  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8          | 50       | 100 | 100 | 0  | 25  | 50  | 100 | 25        | 25 | 75 | 0  | 0  | 0   | 50  | 0         | 0 | 50 | 0  | 0 | 0  | 0   | 25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9          | 25       | 25  | 75  | 51 | 25  | 25  | 50  | 0         | 0  | 25 | 1  | 0  | 0   | 0   | 0         | 0 | 0  | 0  | 0 | 1  | 0   | 0  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

b)

| Accidents: | 0-1 year |     |    |    |     |     |     | 1-5 years |    |    |    |    |     |    | > 5 years |    |    |    |    |    |    |    |   |   |   |   |   |   |   |   |   |   |
|------------|----------|-----|----|----|-----|-----|-----|-----------|----|----|----|----|-----|----|-----------|----|----|----|----|----|----|----|---|---|---|---|---|---|---|---|---|---|
|            | k        | l   | m  | n  | o   | p   | q   | k         | l  | m  | n  | o  | p   | q  | k         | l  | m  | n  | o  | p  | q  |    |   |   |   |   |   |   |   |   |   |   |
| 1          | 75       | 50  | 50 | 1  | 50  | 25  | 50  | 25        | 0  | 25 | 1  | 25 | 0   | 25 | 25        | 0  | 0  | 1  | 0  | 0  | 0  | 25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |   |
| 2          | 75       | 100 | 75 | 0  | 50  | 50  | 50  | 25        | 50 | 50 | 1  | 0  | 25  | 25 | 25        | 0  | 0  | 1  | 0  | 0  | 0  | 0  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |   |
| 3          | 75       | 75  | 50 | 97 | 75  | 75  | 75  | 25        | 25 | 25 | 0  | 25 | 25  | 50 | 0         | 0  | 0  | 1  | 0  | 0  | 0  | 50 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |   |
| 4          | 75       | 75  | 50 | 24 | 75  | 75  | 50  | 50        | 0  | 25 | 1  | 25 | 25  | 0  | 25        | 0  | 0  | 1  | 0  | 0  | 0  | 0  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |   |
| 5          | 75       | 100 | 75 | 24 | 75  | 50  | 50  | 50        | 25 | 50 | 0  | 25 | 25  | 25 | 25        | 25 | 0  | 25 | 1  | 0  | 0  | 0  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |   |
| 6          | 25       | 0   | 50 | 0  | 0   | 0   | 50  | 0         | 0  | 25 | 0  | 0  | 0   | 25 | 0         | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |   |
| 7          | 100      | 100 | 75 | 97 | 100 | 100 | 100 | 75        | 75 | 50 | 74 | 75 | 100 | 75 | 75        | 50 | 50 | 72 | 50 | 50 | 75 | 0  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8          | 25       | 75  | 75 | 23 | 25  | 25  | 100 | 0         | 25 | 50 | 1  | 0  | 0   | 50 | 0         | 0  | 25 | 1  | 0  | 0  | 0  | 50 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9          | 25       | 0   | 75 | 0  | 0   | 0   | 50  | 0         | 0  | 25 | 0  | 0  | 0   | 25 | 0         | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

Tables 7a and b show that the judgements of the validation set panel are generally more consistent than those made by the training set panel. Apart from this, the same trend in judgements can be seen as for the training set, with reduced effects in a long-term perspective. The only exception was accident 7 (where 436 tonnes of chlorobenzene was spilled in a coastal area, close to the sea), which was judged to cause medium or large effects in the long-term perspective for the two sets of responses addressed above. This is also clearly visible in the score plot in Figure 21a. The same trend could also be seen for the other responses, see Table 8 below, which summarises the calculated medians of the judgements.

**Table 8.** The overall judgements, expressed as medians, for each accident and response in (a) the training set and (b) the validation set.

a)

| Accidents: | 1A  |     |    | 1B  |     |    | 1C  |     |    | 2A  |     |    | 2B  |     |    | 3A  |     |    | 3B  |     |    | 4   |     |    | 5   |     |    |
|------------|-----|-----|----|-----|-----|----|-----|-----|----|-----|-----|----|-----|-----|----|-----|-----|----|-----|-----|----|-----|-----|----|-----|-----|----|
|            | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 |
| 1          | 75  | 50  | 25 | 32  | 25  | 15 | 75  | 51  | 40 | 51  | 33  | 25 | 51  | 24  | 11 | 96  | 84  | 74 | 55  | 37  | 25 | 15  | 9   | 3  | 75  | 50  | 40 |
| 2          | 85  | 71  | 48 | 49  | 25  | 16 | 70  | 43  | 26 | 69  | 38  | 17 | 53  | 31  | 7  | 95  | 73  | 25 | 92  | 49  | 25 | 87  | 25  | 8  | 87  | 46  | 16 |
| 3          | 90  | 57  | 25 | 50  | 25  | 6  | 75  | 43  | 25 | 74  | 45  | 22 | 68  | 29  | 6  | 77  | 50  | 25 | 74  | 37  | 11 | 26  | 11  | 2  | 94  | 37  | 8  |
| 4          | 75  | 25  | 4  | 49  | 11  | 5  | 56  | 5   | 5  | 50  | 25  | 3  | 41  | 12  | 5  | 26  | 10  | 9  | 50  | 13  | 10 | 4   | 2   | 3  | 49  | 19  | 4  |
| 5          | 55  | 15  | 2  | 35  | 6   | 3  | 26  | 9   | 3  | 36  | 14  | 3  | 38  | 10  | 4  | 25  | 11  | 3  | 26  | 10  | 3  | 4   | 3   | 2  | 37  | 3   | 1  |
| 6          | 83  | 37  | 9  | 25  | 6   | 2  | 48  | 8   | 4  | 74  | 4   | 4  | 25  | 9   | 4  | 83  | 25  | 5  | 74  | 25  | 6  | 98  | 25  | 3  | 82  | 14  | 5  |
| 7          | 40  | 25  | 5  | 26  | 6   | 3  | 52  | 24  | 4  | 23  | 6   | 4  | 48  | 6   | 3  | 25  | 4   | 3  | 25  | 8   | 6  | 61  | 5   | 3  | 50  | 24  | 3  |
| 8          | 60  | 25  | 7  | 26  | 10  | 2  | 71  | 11  | 6  | 29  | 25  | 5  | 35  | 5   | 4  | 22  | 4   | 3  | 25  | 7   | 6  | 6   | 1   | 1  | 38  | 12  | 2  |
| 9          | 25  | 4   | 3  | 13  | 5   | 4  | 57  | 24  | 16 | 18  | 3   | 2  | 25  | 13  | 4  | 31  | 25  | 5  | 18  | 4   | 2  | 3   | 1   | 2  | 6   | 4   | 4  |

b)

| Accidents: | 1A  |     |    | 1B  |     |    | 1C  |     |    | 2A  |     |    | 2B  |     |    | 3A  |     |    | 3B  |     |    | 4   |     |    | 5   |     |    |
|------------|-----|-----|----|-----|-----|----|-----|-----|----|-----|-----|----|-----|-----|----|-----|-----|----|-----|-----|----|-----|-----|----|-----|-----|----|
|            | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 | 0-1 | 1-5 | >5 |
| 1          | 75  | 25  | 0  | 75  | 25  | 0  | 25  | 0   | 0  | 75  | 25  | 0  | 50  | 2   | 0  | 75  | 50  | 5  | 50  | 25  | 0  | 50  | 13  | 0  | 75  | 25  | 0  |
| 2          | 75  | 25  | 0  | 75  | 50  | 0  | 50  | 25  | 0  | 75  | 50  | 0  | 75  | 25  | 0  | 75  | 50  | 25 | 50  | 25  | 0  | 50  | 0   | 0  | 75  | 25  | 0  |
| 3          | 75  | 25  | 0  | 75  | 50  | 0  | 50  | 25  | 0  | 75  | 25  | 0  | 75  | 50  | 0  | 50  | 25  | 0  | 75  | 25  | 0  | 25  | 0   | 0  | 75  | 25  | 0  |
| 4          | 75  | 25  | 0  | 75  | 25  | 0  | 25  | 1   | 0  | 75  | 25  | 0  | 50  | 25  | 0  | 50  | 25  | 0  | 75  | 25  | 0  | 25  | 0   | 0  | 50  | 0   | 0  |
| 5          | 97  | 25  | 0  | 75  | 25  | 1  | 50  | 1   | 0  | 75  | 25  | 0  | 75  | 25  | 0  | 75  | 50  | 25 | 75  | 25  | 0  | 50  | 0   | 0  | 75  | 50  | 0  |
| 6          | 25  | 0   | 0  | 25  | 0   | 0  | 1   | 0   | 0  | 25  | 0   | 0  | 25  | 0   | 0  | 25  | 0   | 0  | 0   | 0   | 0  | 1   | 0   | 0  | 0   | 0   | 0  |
| 7          | 100 | 75  | 75 | 100 | 73  | 50 | 50  | 25  | 9  | 100 | 75  | 50 | 75  | 50  | 25 | 75  | 75  | 50 | 100 | 75  | 50 | 50  | 2   | 0  | 100 | 72  | 50 |
| 8          | 50  | 25  | 0  | 50  | 25  | 0  | 25  | 0   | 0  | 25  | 0   | 0  | 25  | 0   | 0  | 75  | 25  | 0  | 25  | 1   | 0  | 0   | 0   | 0  | 25  | 0   | 0  |
| 9          | 25  | 0   | 0  | 25  | 0   | 0  | 25  | 0   | 0  | 25  | 0   | 0  | 25  | 0   | 0  | 25  | 0   | 0  | 0   | 0   | 0  | 50  | 0   | 0  | 12  | 0   | 0  |

The *short term* perspective judgements (0-1 year; Table 8a) show that the accidents in the TS represent all the different effect levels (ELs) for responses 1A, 1C, 3B, 4 and 5. However, the accidents do not represent all ELs for responses 2A and 2B (no accidents in the EL76-100% range), 3A (no accidents in the EL 51-75% range), and 1B (no accidents in the EL 51-100% range). The results for the short-term perspective for the validation set, Table 8b, shows that the accidents in the VS represent all the different effect levels for responses 1A, 1B, 3B and 5. However, the accidents do not represent all effect levels for responses 2B and 3A (no accidents in the EL 76-100% range), 2A (no accidents in the EL 51-75% range), 1B and 4 (no accidents in the EL 51-100% range). Notably, the judgements of response 4 differ for the training and validation sets. In the training set the accidents

represent the EL well with respect to responses 4, while the accidents in the validation set do not represent the higher EL.

The judgements for the *medium-* and *long-term* perspective (1-5 years and > 5 years) for the TS in Table 8a do not include all the different levels since all of the accidents were mainly judged to have caused little or no environmental effect over these time periods. This may be due either to the experts finding it hard to judge effects for such a long period of time, or judging that there would not be any residual effects in the environment after a year. Similar results can be seen for the VS in Table 8b. As already mentioned with respect to Table 7, it can be clearly seen that accident 7 differs from the others in the validation set in the sense that it is the only accident judged to cause medium or large effects for almost all responses in the long term. This can be explained by the huge amount of chemical spilled in this particular accident. Overall, the results show that accidents in the training and validation sets cover the effect levels quite well for up to a year, even if the responses do not span all four of the effect levels.

## 6.2 Summary

The results presented in Paper II showed in general that the effects on animal life, vegetation, natural resources, recreational resources and man-made installations could be estimated by the experts, and that questionnaires and expert judgements can be used to collect useful data for the development of EAI. Based on the written comments of the experts, they clearly found it difficult to make the judgements, especially with respect to residual effects more than a year after the accidents (1-5 years and > 5 years). Naturally, long-term effects are difficult to judge because of the complex nature of environmental effects. This could also explain why the judgements differed in relative effect level between the experts, although they generally pointed in the same direction.

The judgements in this study (Paper IV) could not be considered to be “true”, but they do provide rough estimates for planning, prevention and implementation of decontamination steps after chemical accidents. Even more importantly, the measures taken after a chemical accident is built upon judgements such as these nowadays. The overall conclusion is that it would be possible to use such judgements as estimates of environmental effects in the next modelling step, since they all give similar indications, although they were far from unanimous in detail.

## 7 Relating accident descriptors to expert judgements

Improvement of the original EAI, hereafter called EAI<sub>old</sub>, required more knowledge about the weight the new variables should be given (i.e. their relative influence) and understanding about how to incorporate the acquired information into the model. To investigate these issues, the variables were mathematically related to the responses obtained (Paper IV), i.e. the judgements of the environmental effects of the chemical accidents (which are more fully described in Chapter 6). As discussed in Chapter 6, the responses were correlated, and the effects declined with time, i.e. the largest effects were judged to have occurred after 0-1 years, and to have become smaller in the longer term (Figure 21 in Chapter 6). As expected, the experts found it difficult to judge the environmental effects after more than a year, and therefore only the first time interval was modelled.

To get comparable measures of the judgements between the two expert panels the median judgements in each group were used (y-variables in Table 9). Consequently, each accident was assigned a median value for each response to be used in the modelling. The chemical accidents were described by 10 variables, consisting of chemical and site-specific properties (x-variables in Table 9).

**Table 9.** Chemical and site-specific properties<sup>13</sup> of the accidents described, and the median responses, i.e. medians of the expert judgements.

| Accident: | x-variables          |          |          |           |              |                          |            |            |           |          | y-variables                                |           |           |           |           |           |           |          |          |
|-----------|----------------------|----------|----------|-----------|--------------|--------------------------|------------|------------|-----------|----------|--|-----------|-----------|-----------|-----------|-----------|-----------|----------|----------|
|           | Chemical properties  |          |          |           |              | Site-specific properties |            |            |           |          | Expert judgements of environmental effects |           |           |           |           |           |           |          |          |
|           | <i>P<sub>v</sub></i> | <i>v</i> | <i>D</i> | <i>Sw</i> | <i>m/Tox</i> | <i>DNW</i>               | <i>DGS</i> | <i>SGS</i> | <i>K'</i> | <i>n</i> | <i>1A</i>                                  | <i>1B</i> | <i>1C</i> | <i>2A</i> | <i>2B</i> | <i>3A</i> | <i>3B</i> | <i>4</i> | <i>5</i> |
| TS1       | 0.5                  | 2.75     | 820      | 0.1       | 9,5E+09      | 100                      | 5          | 1          | 3         | 35       | 75   | 75        | 32        | 51        | 51        | 96        | 55        | 15       | 75       |
| TS2       | 0.5                  | 2.75     | 820      | 0.1       | 9,5E+09      | 5                        | 0.2        | 1          | 1         | 15       | 85   | 70        | 49        | 69        | 53        | 95        | 92        | 87       | 87       |
| TS3       | 70                   | 1        | 750      | 0.01      | 7,8E+09      | 100                      | 0.01       | 1          | 3         | 33       | 90   | 75        | 50        | 74        | 68        | 77        | 74        | 26       | 94       |
| TS4       | 70                   | 1        | 750      | 0.01      | 7,8E+09      | 2                        | 1.87       | 0.5        | 1         | 43       | 75   | 56        | 49        | 50        | 41        | 26        | 50        | 4        | 49       |
| TS5       | 12.8                 | 0.8      | 790      | 90        | 2,7E+06      | 125                      | 33         | 1          | 1         | 55       | 55   | 26        | 35        | 36        | 38        | 25        | 26        | 4        | 37       |
| TS6       | 0.05                 | 3.2      | 1070     | 8         | 2,7E+10      | 4                        | 4.1        | 0.5        | -         | -        | 83   | 48        | 25        | 74        | 25        | 83        | 74        | 98       | 82       |
| TS7       | 1.2                  | 1        | 880      | 0.007     | 2,7E+08      | 25                       | 23         | 0.5        | 3         | 33       | 40   | 52        | 26        | 23        | 48        | 25        | 25        | 61       | 50       |
| TS8       | 0.6                  | 0.9      | 910      | 0.01      | 6,6E+09      | 1                        | 3.1        | 1          | 3         | 33       | 60   | 71        | 26        | 29        | 35        | 22        | 25        | 6        | 38       |
| TS9       | -                    | 2.25     | 1370     | 0.001     | 2,6E+05      | 200                      | 1.5        | 0.5        | 1         | 15       | 25   | 57        | 13        | 18        | 25        | 31        | 18        | 3        | 6        |
| VS1       | 0.1                  | 1.5      | 808      | 0.1       | 7,8E+09      | 15                       | 1.5        | 1          | 3         | 35       | 75   | 75        | 25        | 75        | 50        | 75        | 50        | 50       | 75       |
| VS2       | 0.5                  | 2.75     | 820      | 0.1       | 1,4E+10      | 7                        | 0.35       | 1          | 1         | 15       | 75   | 75        | 50        | 75        | 75        | 75        | 50        | 50       | 75       |
| VS3       | 0.5                  | 2.75     | 820      | 0.1       | 5,0E+09      | 5                        | 8          | 1          | 1         | 55       | 75   | 75        | 50        | 75        | 75        | 50        | 75        | 25       | 75       |
| VS4       | 70                   | 1        | 750      | 0.01      | 5,8E+09      | 25                       | 0.01       | 1          | 2         | 35       | 75   | 75        | 25        | 75        | 50        | 50        | 75        | 25       | 50       |
| VS5       | 70                   | 1        | 750      | 0.01      | 7,2E+09      | 2                        | 16         | 1          | 1         | 43       | 97   | 75        | 50        | 75        | 75        | 75        | 75        | 50       | 75       |
| VS6       | 4.2                  | 3        | 790      | 90        | 7,9E+04      | 300                      | 2          | 1          | 2         | 35       | 25   | 25        | 1         | 25        | 25        | 25        | 1         | 1        | 1        |
| VS7       | 1.2                  | 1        | 1110     | 0.05      | 2,1E+11      | 30                       | 2.3        | 1          | 1         | 15       | 100  | 100       | 50        | 100       | 75        | 75        | 100       | 50       | 100      |
| VS8       | 12                   | 1        | 930      | 0.02      | 1,7E+09      | 7                        | 7.6        | 0.5        | 2         | 35       | 50   | 50        | 25        | 25        | 25        | 75        | 25        | 1        | 25       |
| VS9       | 4.3                  | 1.5      | 1220     | 90        | 8,7E+07      | 30                       | 3.2        | 0.5        | 1         | 15       | 25   | 25        | 25        | 25        | 25        | 25        | 1         | 50       | 12       |

<sup>13</sup> See abbreviations, Page *ii*.

## 7.1 PLS modelling

A mathematical relationship was developed between the x-variables and the judgements of nine responses (1A-5) by the expert panel (y-variables<sup>14</sup>), as shown in Figure 22. The mathematical model was obtained using PLS and the new PLS model was then used to derive variable information on the weight and importance of the x-variables.

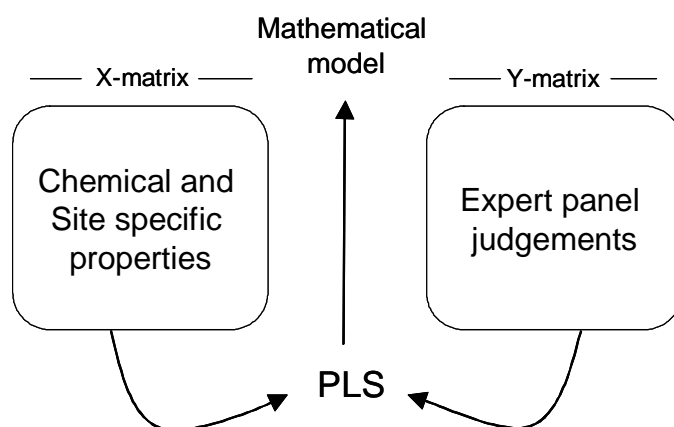


Figure 22. Schematic diagram of the modelling process.

The dataset of chemical accidents was initially divided in two subsets; a training set (TS) and a validation set (VS), in order to allow external validation of a model built on the TS. However, during the first modelling phase it was found that there were too few accidents in the TS to represent the variation in the VS and to build a model that covered a broad spectrum of chemical accident situations. Therefore, we decided to consider both the training and validation sets as a single, combined set for the modelling and to restrict the validation procedures to internal validation (cross-validation).

<sup>14</sup> **1A**: effects on animal life in the aquatic environment ; **1B**: effects on ground-living animals and micro organisms; **1C**: effects on animals in the terrestrial (above-ground) environment; **2A**: effects on vegetation in the aquatic environment; **2B**: effects on vegetation in the terrestrial environment; **3A**: effects on the potential for using groundwater and surface water for drinking water; **3B**: effects on the potential for using land and water for economic activities, e.g. growing crops and forestry, commercial fishing and building; **4**: effects on vital installations, such as wells, cables, sewage systems, and water treatment plants etc; **5**: effects on the potential for recreational activities, such as fishing (angling), walking, trekking and swimming.

The modelling resulted in a one-component PLS model for the time interval 0-1 year with  $R^2$  and  $Q^2$  values of 0.758 and 0.648, respectively. This model was obtained through several steps (described in more detail below) in which one accident (T8), three responses (1C, 2B and 4) and three property variables ( $K'$ ,  $n$  and  $v$ ) were excluded from the calculations, for the following reasons.

Firstly, accident T8 was found to be an outlier in its relation between X and Y (see Paper IV), and hence was excluded. Secondly, it had already been observed (Paper III) that response 4 (effects on vital installations) behaved differently from the other responses (Figure 21, Chapter 6) and so was also excluded, resulting in a two component model with  $R^2$  and  $Q^2$  values of 0.749 and 0.518, respectively. Thirdly, responses 1C (effects on animals in the terrestrial environment) and 2B (effects on vegetation in the terrestrial environment), proved to have a lower predictive capacity ( $Q^2$ ; see Paper IV) than the other responses and to investigate if the predictive power of the model would be better without these responses they were excluded, resulting in a model with  $R^2$  and  $Q^2$  of 0.756 and 0.593, respectively. Finally, three property descriptors ( $K'$ , hydraulic conductivity;  $n$ , porosity; and  $v$ , viscosity), were excluded since they were of low importance for the model, as shown in the  $VIP^{15}$ -plot in Figure 25, and the final model,  $EAI_{new}$  was calculated as described above.

It is of great importance to point out that the excluded variables are of low significance only for  $EAI_{new}$  and its proposed usage, and that these chemical and site-specific properties together with the responses are still important factors to consider in every type of chemical accident.

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<sup>15</sup> The Variable Influence on Projection parameter (VIP) shows how each variable influences the model.

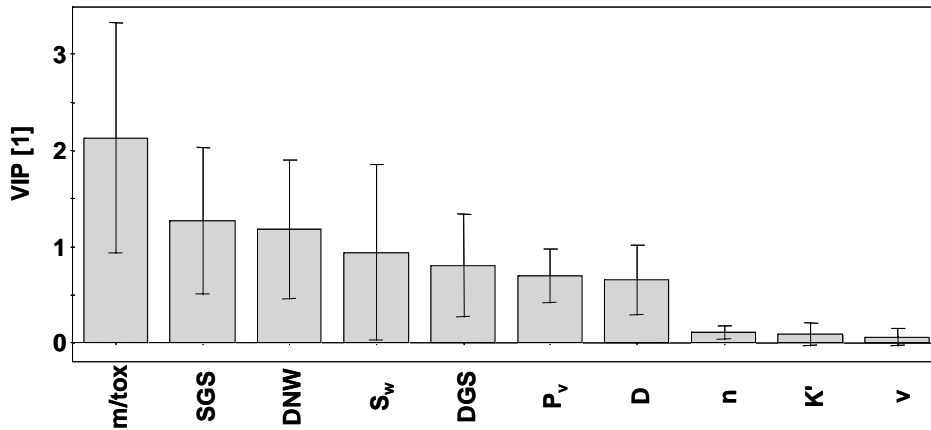


Figure 23. Variable of Importance Plot (VIP) plot of the x-variables.

## 7.2 $EAI_{new}$ in relation to $EAI_{old}$

To investigate the weight and importance of the accident-describing variables in the new model in relation to the variables in  $EAI_{old}$ ,  $EAI_{new}$  can be re-expressed as a regression model. The PLS analysis showed that the pattern of explained variance is similar among all responses (Paper IV). This means that the responses are similar in character and, generally, one response can be selected to represent the others. Therefore, response 2A is used as an example to study the feasibility of such an approach. A regression model was expressed through the use of regression coefficients derived from  $EAI_{new}$  for each variable (see Chapter 3).

The result is presented in Eq. 6, in which all the variables are unscaled but transformed (transformations according to Paper IV).

$$\begin{aligned}
 EAI_{new} = & 18,9 + \underbrace{[7,1(P_v)^{-0,25} + 8,7 \cdot 10^6(D)^{-2} - 3,2 \log S_w]}_{\text{Chemical property variables}} + 0,07(m/Tox)^{0,25} \\
 & - \underbrace{[6,8(DNW)^{0,25} - 7,4(DGS)^{0,25} + 27,9SGS]}_{\text{Site-specific property variables}}
 \end{aligned}
 \tag{Eq. 6}$$

To compare the relative weights in the model of the variable  $m/Tox$  and two groups of variables – the chemical properties ( $P_v$ ,  $D$  and  $S_w$ ) and the site-specific properties ( $DNW$ ,  $DGS$  and  $SGS$ ) – each variable and the sum of

these groups were calculated for the accidents in the dataset according to Eq. 6. The results can be seen in Table 10.

**Table 10.** Calculated variables, and calculated sums of both chemical property variables and site-specific variables, according to  $EAI_{new}$ .

| Accident: | $P_v$ | $D$  | $S_w$ | $m/Tox$ | $DNW$ | $DGS$ | $SGS$ | $\sum$ Chem.prop.var | $\sum$ Site-spec.var |
|-----------|-------|------|-------|---------|-------|-------|-------|----------------------|----------------------|
| TS1       | 8.4   | 12.9 | 3.2   | 21.9    | -21.5 | -11.1 | 27.9  | 24.5                 | -4.7                 |
| TS2       | 8.4   | 12.9 | 3.2   | 21.9    | -10.2 | -4.9  | 27.9  | 24.5                 | 12.8                 |
| TS3       | 2.5   | 15.5 | 6.4   | 20.8    | -21.5 | -2.3  | 27.9  | 24.4                 | 4.1                  |
| TS4       | 2.5   | 15.5 | 6.4   | 20.8    | -8.1  | -8.7  | 14    | 24.4                 | -2.8                 |
| TS5       | 3.8   | 13.9 | -6.3  | 2.8     | -22.7 | -17.7 | 27.9  | 11.4                 | -12.5                |
| TS6       | 15    | 7.6  | -2.9  | 28.4    | -9.6  | -10.5 | 14    | 19.7                 | -6.1                 |
| TS7       | 6.8   | 11.2 | 6.4   | 9       | -15.2 | -16.2 | 14    | 24.4                 | -17.4                |
| TS8       | 8.1   | 10.5 | 6.4   | 20      | -6.8  | -9.8  | 27.9  | 25                   | 11.3                 |
| TS9       | -     | 4.6  | 9.6   | 1.6     | -25.6 | -8.2  | 14    | 14.2                 | -19.8                |
| VS1       | 12.6  | 13.3 | 3.2   | 20.8    | -13.4 | -8.2  | 27.9  | 29.1                 | 6.3                  |
| VS2       | 8.4   | 12.9 | 3.2   | 24.1    | -11.1 | -5.9  | 27.9  | 24.5                 | 10.9                 |
| VS3       | 8.4   | 12.9 | 3.2   | 18.6    | -10.2 | -12.4 | 27.9  | 24.5                 | 5.3                  |
| VS4       | 2.5   | 15.5 | 6.4   | 19.3    | -15.2 | -2.3  | 27.9  | 24.4                 | 10.4                 |
| VS5       | 2.5   | 15.5 | 6.4   | 20.4    | -8.1  | -14.8 | 27.9  | 24.4                 | 5                    |
| VS6       | 5     | 13.9 | -6.3  | 1.2     | -28.3 | -8.8  | 27.9  | 12.6                 | -9.2                 |
| VS7       | 6.8   | 7.1  | 4.2   | 47.4    | -15.9 | -9.1  | 27.9  | 18.1                 | 2.9                  |
| VS8       | 3.8   | 10.1 | 5.4   | 14.2    | -11.1 | -12.3 | 14    | 19.3                 | -9.4                 |
| VS9       | 4.9   | 5.8  | -6.3  | 6.8     | -15.9 | -9.9  | 14    | 4.4                  | -11.8                |

The results show that  $SGS$  is the most important of the calculated variables, followed by  $m/Tox$ ,  $DNW$ ,  $D$ ,  $DGS$ ,  $P_v$  and  $S_w$ . The variables in the two groups were summed to compare their importance. In general the  $EAI_{new}$  is more strongly influenced by the chemical variable group and single variable  $m/Tox$  than the site-specific variable group (these groups and the variable  $m/Tox$  are coloured grey in the table).

Regarding how each variable influence the magnitude of  $EAI_{new}$  compared to how they influenced  $EAI_{old}$ , the results show that  $m/Tox$  (compared to  $Am$  and  $Tox$ ),  $DNW$ ,  $DGS$  and  $SGS$  (all of which contribute to the variable  $Sur$ ) influenced the magnitude of  $EAI$  in the same way in both the old and new models. For example: high values of  $m/Tox$  (due to very large amounts of the chemicals involved, or very toxic chemicals, or both) give high values when calculated in  $EAI_{new}$ , and also high values for  $Am$  and  $Tox$ , in Tables

6 and 8 in Appendix I, for the calculation of  $EAI_{old}$ . High values mean, for both indices, large effects in the environment.

However, the influence of one variable,  $S_w$ , on the two models is qualitatively different. Low water solubility gives a high value in  $EAI_{new}$  and a low value in  $EAI_{old}$ , which means that highly soluble chemicals give (according to Table 9 in Appendix I) the highest value calculating  $EAI_{old}$  while highly soluble chemicals have a negative influence on the magnitude of  $EAI_{new}$ . This difference between the models is probably due to the fact that  $EAI_{old}$  contained inorganic chemicals that could both be highly soluble and toxic. The difference can also be due to the judgements related to  $EAI_{new}$ , since the experts probably considered the largest environmental effects to be associated with accidents involving chemicals with low water solubility. For variables  $P_v$  and  $D$ , which were added to  $EAI_{new}$  a high vapour pressure ( $P_v$ ) and a high density gives low values in  $EAI_{new}$  (indicating small effects in the environment) and vice versa.

### 7.3 *Classes*

$EAI_{old}$  was developed for use with a three-category risk scale, with classes 0-100, 100-500 and more than 500. Each category or class was associated with specific recommendations regarding further investigations and measures that should be taken for the described accident scenario. This approach was satisfactory since the purpose of the EAI is to give guidelines about measures that should be taken, rather than exact risk values. The new model,  $EAI_{new}$ , is mainly based on the accident-describing variables of  $EAI_{old}$ , with a few additional variables. One purpose of this study was to compare the original  $EAI_{old}$  and  $EAI_{new}$  to see which descriptors were important and decide the weights they should be given in a final model.

To facilitate such a comparison, the  $EAI_{new}$  also has to use categories or classes. One possibility would have been to use the same division of effect levels as used in the questionnaires i.e. 0-25% = no/small effects; 25-50 = small to moderate effects; 50-75 = moderate to large effects and 75-100 = very large effects. However, the classification associated with  $EAI_{old}$  was based on three categories and the initial evaluation of  $EAI_{old}$  (see Chapter 4) indicated that the limits for these categories worked well. Given this, and the fact that accidents should be neither underestimated nor overestimated, the following classification scale was proposed.

- Class I:** 0-33% for small to moderate effects
- Class II:** 34-74% for moderate to large effects
- Class III:** 75-100% for large to very large effects

Using this new classification scale,  $EAI_{new}$  can be compared to  $EAI_{old}$ .

#### 7.4 Observed vs predicted effects

To evaluate the PLS model the estimated predictions of model  $EAI_{new}$  were analysed. In Table 11 the observed versus the estimated (or predicted) values for each accident and response can be seen, the classified accidents being coloured grey. It has to be remembered that there is a confidence interval for every observed and, hence, every predicted response value. In Table 11 borderline response values (defined as those within a confidence interval of +/- 2 of the limit between two classes) are marked with circles, and underestimated response values are marked with squares.

**Table 11.** Observed and estimated (predicted) values of model  $EAI_{new}$ .

| Accidents: | 1A <sub>obs</sub> | 1A <sub>pred</sub> | 1B <sub>obs</sub> | 1B <sub>pred</sub> | 2A <sub>obs</sub> | 2A <sub>pred</sub> | 3A <sub>obs</sub> | 3A <sub>pred</sub> | 3B <sub>obs</sub> | 3B <sub>pred</sub> | 5 <sub>obs</sub> | 5 <sub>pred</sub> |
|------------|-------------------|--------------------|-------------------|--------------------|-------------------|--------------------|-------------------|--------------------|-------------------|--------------------|------------------|-------------------|
| T1         | 75                | 71                 | 75                | 65                 | 51                | 61                 | 96                | 62                 | 55                | 57                 | 75               | 63                |
| T2         | 85                | 88                 | 70                | 79                 | 69                | 78                 | 95                | 77                 | 92                | 77                 | 87               | 84                |
| T3         | 90                | 78                 | 75                | 71                 | 74                | 68                 | 77                | 68                 | 74                | 66                 | 94               | 72                |
| T4         | 75                | 72                 | 56                | 65                 | 50                | 61                 | 26                | 62                 | 50                | 57                 | 49               | 63                |
| T5         | 55                | 32                 | 26                | 33                 | 36                | 20                 | 25                | 29                 | 26                | 10                 | 37               | 16                |
| T6         | 83                | 72                 | 48                | 65                 | 74                | 61                 | 83                | 62                 | 74                | 57                 | 82               | 63                |
| T7         | 40                | 47                 | 52                | 45                 | 23                | 35                 | 25                | 41                 | 25                | 27                 | 50               | 33                |
| T9         | 25                | 32                 | 57                | 32                 | 18                | 19                 | 31                | 28                 | 18                | 9                  | 6                | 15                |
| V1         | 75                | 85                 | 75                | 76                 | 75                | 75                 | 75                | 74                 | 50                | 74                 | 75               | 80                |
| V2         | 75                | 89                 | 75                | 79                 | 75                | 79                 | 75                | 77                 | 50                | 78                 | 75               | 84                |
| V3         | 75                | 78                 | 75                | 70                 | 75                | 68                 | 50                | 68                 | 75                | 65                 | 75               | 71                |
| V4         | 75                | 83                 | 75                | 75                 | 75                | 73                 | 50                | 72                 | 75                | 71                 | 50               | 77                |
| V5         | 97                | 79                 | 75                | 71                 | 75                | 69                 | 75                | 69                 | 75                | 66                 | 75               | 73                |
| V6         | 25                | 35                 | 25                | 35                 | 25                | 23                 | 25                | 31                 | 0                 | 13                 | 0                | 19                |
| V7         | 100               | 97                 | 100               | 86                 | 100               | 88                 | 75                | 84                 | 100               | 88                 | 100              | 94                |
| V8         | 50                | 54                 | 50                | 51                 | 25                | 43                 | 75                | 48                 | 25                | 36                 | 25               | 42                |
| V9         | 25                | 30                 | 25                | 31                 | 25                | 18                 | 25                | 27                 | 0                 | 7                  | 12               | 13                |

The fact that many of the non-classified response values (41) were borderline values (26) and a few (7) were underestimated is satisfactory. Even if some of the response values are close to class limits, and therefore the classification has a fairly high degree of uncertainty, these results show

that the model gives class predictions that are at least close to corresponding observed response values.

It is also clear from the data in Table 11 that the highest number of accidents (71%) can be classified by responses 1A (effects on water-living organisms) and 3B (effects on the use of natural resources. Similarly, the lowest number of accidents can be classified according to responses 3A and 5 (53% and 47% respectively), while 59% can be classified by responses 1B and 2A. Summarising the distribution of the accidents into classes based on the responses, seven were classified as Class II, while Class I and III included four and six accidents, respectively. This is very close to the  $EAI_{old}$  categories calculated for the same accidents, since eight of them were placed in category 100-500, four in category 0-100, and five in category >500.

### *7.5 Prediction of responses for 37 chemical accidents*

Despite the fact that no external validation set could be used for the predictions,  $EAI_{new}$  was used to predict responses for 37 chemical accidents. These 37 accidents were part of the dataset considered in the selection procedure (Chapter 5). The responses related to these accidents are not known, since they were not part of the expert panel study. Table 12 shows the results of the predictions.

**Table 12.** Predictions of responses for 37 accidents (more information on these accidents can be found in Chapter 2, Table 1). The table shows the predicted response for the six responses 1A – 5, the Model membership Probability (MP) with a 95% confidence level, the distance to the model (DModX), and the class of each accident according to the classification scale in Section 7.3.

| Accidents | MP   | DModX | 1A  | 1B  | 2A  | 3A  | 3B  | 5   | Class |
|-----------|------|-------|-----|-----|-----|-----|-----|-----|-------|
| 1         | 0.76 | 0.74  | 83  | 75  | 73  | 73  | 72  | 78  | II    |
| 2         | 0.45 | 1.02  | 77  | 70  | 67  | 68  | 65  | 71  | II    |
| 4         | 0.65 | 0.84  | 95  | 84  | 85  | 83  | 85  | 92  | III   |
| 5         | 0.62 | 0.87  | 80  | 72  | 70  | 70  | 67  | 73  | II    |
| 6         | 0.15 | 1.45  | 39  | 38  | 27  | 34  | 18  | 24  | I     |
| 7         | 0.88 | 0.61  | 73  | 67  | 63  | 64  | 59  | 65  | II    |
| 8         | 0.95 | 0.49  | 108 | 95  | 99  | 94  | 101 | 108 | III   |
| 10        | 1.00 | 0.28  | 85  | 76  | 75  | 74  | 74  | 80  | III   |
| 11        | 0.86 | 0.64  | 59  | 55  | 48  | 52  | 42  | 48  | II    |
| 12        | 0.96 | 0.47  | 81  | 73  | 71  | 71  | 69  | 75  | II    |
| 13        | 0.97 | 0.44  | 72  | 66  | 62  | 63  | 58  | 64  | II    |
| 14        | 0.67 | 0.83  | 58  | 54  | 48  | 51  | 42  | 48  | II    |
| 17        | 1.00 | 0.24  | 85  | 76  | 75  | 74  | 74  | 80  | III   |
| 18        | 0.38 | 1.10  | 83  | 75  | 73  | 73  | 72  | 78  | III   |
| 19        | 0.13 | 1.50  | 55  | 51  | 43  | 48  | 37  | 43  | II    |
| 20        | 0.06 | 1.78  | 36  | 36  | 24  | 32  | 15  | 20  | I     |
| 22        | 0.87 | 0.63  | 80  | 72  | 70  | 70  | 67  | 73  | II    |
| 23        | 0.04 | 1.93  | 9   | 14  | -4  | 9   | -18 | -12 | I     |
| 24        | 0.43 | 1.04  | 65  | 60  | 54  | 57  | 49  | 55  | II    |
| 25        | 0.07 | 1.71  | 134 | 116 | 126 | 116 | 133 | 139 | III   |
| 26        | 0.93 | 0.54  | 65  | 60  | 55  | 57  | 50  | 56  | II    |
| 27        | 0.42 | 1.05  | 78  | 70  | 68  | 68  | 65  | 71  | II    |
| 28        | 0.88 | 0.61  | 71  | 64  | 60  | 62  | 56  | 62  | II    |
| 29        | 0.70 | 0.80  | 80  | 72  | 70  | 69  | 67  | 73  | II    |
| 33        | 0.47 | 1.01  | 56  | 52  | 45  | 49  | 38  | 44  | II    |
| 34        | 0.33 | 1.16  | 84  | 76  | 74  | 73  | 73  | 79  | II    |
| 36        | 0.15 | 1.45  | 49  | 47  | 37  | 43  | 30  | 36  | II    |
| 37        | 0.43 | 1.05  | 63  | 58  | 52  | 55  | 47  | 53  | II    |
| 38        | 0.54 | 0.94  | 68  | 62  | 57  | 59  | 53  | 59  | II    |
| 39        | 0.75 | 0.75  | 78  | 71  | 68  | 68  | 66  | 72  | II    |
| 40        | 0.74 | 0.76  | 80  | 72  | 69  | 69  | 67  | 73  | II    |
| 43        | 0.45 | 1.03  | 102 | 90  | 92  | 88  | 94  | 100 | III   |
| 46        | 0.83 | 0.67  | 60  | 56  | 49  | 53  | 44  | 50  | II    |
| 51        | 0.47 | 1.00  | 49  | 47  | 38  | 43  | 30  | 36  | II    |
| 52        | 0.70 | 0.77  | 56  | 52  | 45  | 49  | 39  | 45  | II    |
| 53        | 0.30 | 1.19  | 31  | 32  | 19  | 28  | 9   | 15  | I     |
| 54        | 0.86 | 0.63  | 41  | 40  | 29  | 36  | 20  | 26  | I     |

The Model membership Probability, MP, values show that most accidents, at a 95% confidence level, belong to the model. This finding shows that the accidents selected to build the model ( $EAI_{new}$ ) adequately covered all of the accidents in the original dataset. Only one accident, No 23, has a model membership probability lower than 5%. This accident also shows a DModX value (1.93) above the critical limit for a 95% confidence level (1.838), which means that it is regarded as an outlier and does not belong to the

model. In Chapter 5, Figure 18, accident 23 is also shown to be a weak outlier in the score plot when site-specific properties are considered.

When all the predicted responses (1A, 1B, 2A, 3A, 3B and 5) are taken into account each accident can be placed in a class according to the classification scale in Section 7.2. The results showed that five accidents were placed in Class I, 25 accidents in Class II, and seven accidents in Class III. This can be regarded as a normal distribution.

### 7.6 *Practical use of $EAI_{new}$*

What are the advantages of  $EAI_{new}$  compared to  $EAI_{old}$ ? Firstly,  $EAI_{new}$  does not require nine tables for its calculation: instead it can be directly calculated from raw data. This is advantageous since the use of tables is not only time consuming, but there is also a risk that wrong values may be taken from the tables when calculating  $EAI_{old}$ . Secondly, the calculated PLS version of  $EAI_{new}$  can estimate effects for all of the included responses, as well as roughly classifying accidents according to the new classification scale. Thirdly, the regression model of  $EAI_{new}$  based on a response, such as the example shown above with response 2A, can easily be calculated by anyone without the ability to perform PLS, especially if pre-calculated values of the chemical properties and toxicity are listed and only the site-specific properties have to be included. It is also very easy to make regression models for all responses in the same way as illustrated for response 2A. Finally, and most importantly, the  $EAI_{new}$  is based on a selected set of representative chemical accidents chosen from a larger and more diverse dataset than  $EAI_{old}$ , and was developed, via this selection, to be as unbiased as possible. This should make the  $EAI_{new}$  safer to use for many different organic chemicals and situations as it covers a broader spectrum of accident scenarios.

These advantages make it possible for authorities, industrial concerns and other interested parties in different parts of Sweden (or any other country) to calculate estimated effects in a standardized way. The only tasks they have to perform in order to make the calculations are to select a site for investigation, and then define the properties of the site (*DNW*, *DGS* and *SGS*) and the amount of chemical “to be spilled”.

## 7.7 Summary

In general, the results of this study (Paper IV) showed that the variable  $m/Tox$  clearly has the largest influence on the models, followed by  $SGS$  (slope of groundwater surface),  $DNW$  (distance to nearest well, lake or watercourse) and  $S_w$  (Water solubility). Descriptors  $DGS$  (distance to groundwater surface),  $D$  (density) and  $P_v$  (vapour pressure) are less influential, and  $K'$  (hydraulic conductivity of the soil),  $n$  (porosity of the soil), and  $\nu$  (viscosity) have little or no influence on the models. These findings can be explained by the relative difficulty for the experts to understand and use the variables, which in turn depends on their familiarity with judging the influence of these variables.

The amount and toxicity of the chemicals involved are easy to understand and analyse, and relevant data are fairly easy to access, which means that the experts are probably trained to use such information.  $SGS$ ,  $DNW$ ,  $S_w$ ,  $DGS$ ,  $D$  and  $P_v$  are also relatively easy to analyse, although it can be harder to find information on some of these descriptors. The viscosity is probably not often used (it is harder to find data on this variable than the other chemically-related variables) and is thus not considered to a large extent in the judgements.

The hydraulic conductivity ( $K'$ ) and porosity ( $n$ ) of the soil were used in an attempt to describe the soil numerically in a way that also gave sufficient information on soil properties that influence the effects of accidents. The results show that these types of variables did not adequately describe the soil properties, and the old system, relying on simple soil variables as outlined in the initial evaluation of the EAI (Chapter 4), may have provided a better way of describing these properties. It is also possible that geology and related variables were difficult to judge because many of the experts lacked formal education in hydrogeology and/or had little experience in judging these variables. This was also confirmed by the interviews with the EHOs (see Chapter 8). Furthermore, this type of information is often difficult to obtain. All these aspects might have led to increased uncertainty in the judgements or caused the experts to pay less attention to these factors.

The response variables 1C, 2B and 4 were found to be less well explained (i.e. had lower  $R^2$  values) by the model and to have lower predictive capacity ( $Q^2$ ). It is possible that the experts found it difficult to judge responses related to the terrestrial environment (1C and 2B) because some important variables for describing these effects are not available in the EAI model and hence also a lack of experience to judge these effects.

One object, accident T8 (involving the spillage of 60 tonnes of styrene in a harbour area), was also removed from the data set as it was considered an outlier in the y-space. One reason for this is that the experts judged T8 to cause effects on vegetation in the aquatic environment (2A) varying from 0-96% (i.e. their opinions of its environmental effects varied greatly). The median value in this case (29%) is a poor description of the actual judgements, so the accident becomes an outlier.

By excluding less important variables and responses a better model,  $EAI_{new}$ , was obtained.  $EAI_{new}$  has the capacity to classify accidents roughly, if combined with the proposed new three-class classification scale. Further, the results of  $EAI_{new}$  showed that

- A regression model of  $EAI_{new}$  (each response), could be obtained based on the regression coefficients of the variables.
- When the contribution of each variable group to  $EAI_{new}$  is calculated, the chemical property variables ( $P_v$ ,  $D$ ,  $S_w$ ) have greater total influence on the magnitude of the  $EAI_{new}$  than the site-specific variables ( $DNW$ ,  $DGS$ ,  $SGS$ ).
- Variables related to water solubility ( $S_w/Sol$ ) have qualitatively different effects on the magnitude of  $EAI_{old}$  and  $EAI_{new}$ .
- The prediction of the accidents with unknown responses showed that  $EAI_{new}$  has been established on a valid base of accident scenarios, showing that the model can already be used at this stage of development.

## 8 Interviews

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### 8.1 Background

An important actor at the chemical accident site is the EHOs representing the EHPDs as also described in Section 1.2. To gain more knowledge of the operational conditions for these persons to be used in the final refinement of the EAI, the EHOs of the 18 selected municipalities were interviewed during the expert panel study (Paper III). The interviews were carried out from April to June 2002 and this Chapter describes the operational conditions of the interviewees at that time.

The EHOs were asked questions about how their organisation handles matters related to chemical accidents, such as preventative work and cooperation at both the local level (i.e. with other departments) and the regional level (i.e. with other municipalities). Other questions asked concerned the kind of knowledge they felt was missing and the kind of help they wanted from authorities. They were also asked to speculate about the kinds of service or tools that could facilitate their work. The objectives of the interviews were to discover the nature of the problems the EHOs may experience during their work in this field, and the kinds of knowledge or service that they felt could assist or improve their work.

The EHPDs varied in size from small departments with 2-4 officers to medium (10-20 officers) and really large departments (50-90 officers). Eight of the interviewed officers were formally educated as environmental officers, five as engineers and four had an older type of environmentally-related education. When the officers described the accident statistics for their municipalities, the numbers varied from a few accidents per year to 15-20 accidents of varying size. The most common were transport accidents and the spilled chemical was mostly a petroleum product. Another common type of accident was due to oil tanks being overfilled in private households. Several of the interviewees had noticed that relatively high frequencies of dangerous goods that were transported through their municipalities originated from Russia, Poland and the Baltic states. They saw accidents involving such vehicles as being especially risky since these states do not apply the same standards and safety routines as Sweden, and the companies handling the chemicals are usually not insured, so the affected municipalities have to pay for any essential decontamination.

## 8.2 *Has the view of chemical accidents changed over the years?*

The general opinion among the interviewees was that views on chemical accidents have changed, and the main reasons for this are that knowledge has increased, legislation has become more stringent and accidents now receive more publicity in the media. This also applies to the FRS, which have improved their awareness of the environmental problems that chemical accidents may cause, according to the EHPDs.

## 8.3 *Organisation related to chemical accidents*

Generally, an FRS or SOS Alarm notifies the EHPD that an accident has occurred, and the officer whose name appears first on the alarm list for handling these kinds of emergencies. The notified officers then discuss with the Incident Commander of the FRS how quickly they want help, or if assistance can be given over the phone. However, almost without exception, the EHO will want to assess the situation on site. Sometimes this can cause problems since they are not on duty in the evenings and at weekends, so they may be far away from the accident site when it occurs. Only one EHPD (in the municipality of Örebro) included in the study (and as far as I know the only one in Sweden) has a 24-hour duty-roster in the same way as the FRS. They are organised in such a way that each officer in the group has a 24-hour duty period every 10<sup>th</sup> week, for which they get paid and also an extra day off. Two departments have a system with emergency duty during the daytime. A few EHPDs have a system in which the head of the department can always be reached through a mini-call service and one department has a system where the officer gets paid extra for the time he or she puts into dealing with each incident. Many of the other interviewed officers have a positive attitude towards systems with 24-hour duty, but the determining factor is financial, as the budgets for the EHPDs are becoming increasingly tight.

In municipalities where the FRS makes the call to the EHPD the personal contacts are of vital importance as they make it much easier to contact the appropriate staff in emergency situations.

All the interviewed EHPDs, except for the smallest, allow two of their officers to attend the accident site in order to minimise disruption to the emergency procedures if one of the officers is later called away on another mission. All EHPDs have a back-up person who can assist at the office to get the necessary information for the officers on site. Many EHPDs have a

special shelf or other place where relevant information, such as information about chemicals, checklists, maps, and equipment is stored for dealing with these types of incidents. For further information on chemicals etc., one EHPD used a local expert based at a local chemical plant, and one used a retired expert. In summary, only a few of the interviewees had personal contacts that they could call for information on chemical compounds and related issues.

Whether or not external experts are commissioned depends on the size of the municipality. Larger cities often have broad competence within the department, while smaller ones may need to turn to consultants. In some cities the policy is that the EHPDs merely point out what needs to be done at accident sites, and parties that caused them are required to clean up. The networks of the environmental officers are very important here, and often personal contacts are used instead of consultants. Furthermore, large industrial concerns often have their own chemical experts and some even have equipment for sampling available if the accident occurs at one of their industrial sites.

#### *8.4 Equipment*

The type of equipment available varies greatly between the EHPDs and neither its extent nor its sophistication is related to the size of the departments. Some EHPDs only take high boots, a lamp, a camera and a note-book to the accident site while others take an advanced emergency kit containing everything from abundant relevant information (e.g. maps, phone lists and instructions) to equipment for sampling. A few EHPDs have special jackets and reflective vests to ensure that they are clearly visible and identifiable at the accident site. A few of the EHPDs have digitalised their maps (showing hydrogeological features, sensitive objects, water catchments, wells etc) and use a GIS tool to process the data. Most of the EHPDs see this as the way that information should be handled everywhere in the future, as it is very convenient to have all the maps in the same place, and integrated in such way that if a specific site is investigated all stored information about it can be accessed simultaneously. However, even if the EHPDs see this as the way forward, not many can currently afford it as it takes significant amounts of resources to build, administer and update such a system.

### *8.5 How well are the accidents managed?*

The general view is that the accidents are handled satisfactorily with respect to the cooperation with the FRS and the decontamination process. Generally, the EHPDs feel that the FRS has trust in them and the FRS often wants support to help make their initial decisions concerning decontamination. However, one officer said that the FRS members want to go home as soon as possible, for financial reasons, and suggested that it would be better if the FRS could take more far-reaching responsibilities for a smooth and careful decontamination process. Further, he thought that communication failures sometimes occurred between the FRS and the EHPD in the phase in which responsibility is transferred from the former to the latter. On the other hand, one officer thought that the FRS was too ambitious in their cleaning-up operations.

Nevertheless, one issue was consistently emphasized; the importance of clear organisation, where the responsibilities of all actors are well defined, before they meet at the accident site, and the key words used were sharing and information.

One issue often mentioned was the role of the insurance companies at the accident sites. Mostly, it was felt that the accidents were smoothly handled, but in some municipalities the EHOs believed that the insurance companies do not always promote speed and efficiency in the decontamination processes. The insurance companies often have directives that do not match the requirements of the EHPDs or companies responsible for cleaning up. Consequently, the EHPDs often feel that there is a conflict between the demands for satisfactory decontamination and the financial imperatives of the insurance companies. During the interviews, for instance, an incident was described in which an insurance company's representative left the accident site when it was discovered that the house owner did not have the proper insurance to cover the situation.

### *8.6 Evaluation of accidents and use of external experts*

In small municipalities there are usually no formal evaluations after chemical accidents, but the EHPD, the FRS and other departments are often located close to one another, and therefore informally exchange information about accidents in their locality. Some of the interviewees from small municipalities said that lots of information was exchanged during joint "fikas" or coffee breaks. In the larger municipalities more serious accidents

are often formally evaluated, and a few authorities carry out such evaluations once or twice a year, sometimes together with neighbouring municipalities. On such occasions, all accidents that have occurred during the year are discussed. However, the most common way to evaluate accidents is for the parties that caused them to present a report on the course of events, actions taken and the environmental effects that were caused.

### 8.7 *Preventative work and cooperation*

Most of the work designed to prevent chemical accidents is done through supervision at industrial plants and legislation. The EHPD can help an industrial plant or sector to prevent chemical accidents and to decrease the effects in case accidents occur by pointing out weak spots in the industrial facility.

Other preventative work can involve protecting water catchment areas and redirection of transport routes for dangerous goods to less sensitive areas. In the municipality of Umeå, such preventative work resulted in the construction of an environmental sensitivity map (*Liljedahl et al 1999*), and through the interviews many of the EHPDs see such approaches as being valuable strategies for preparing maps and other information in the future.

In addition, some preventative work is done through the development of contingency plans, in which chemical accidents are just one of several types of scenario discussed. It is possible that cooperation between the EHPD and other departments may start through such work.

Generally, the EHPDs have good contacts with the FRS, the Technical Department<sup>16</sup> (TD) and the City Planning Department<sup>17</sup> (CPD), but actual (formalised) cooperation is more occasional. With respect to chemical accidents, the main cooperating organisations are the FRS and the TD. Such cooperation may lead to the formation of chemical accident groups, training exercises for handling chemical accidents, the development of checklists, joint inspections at industrial sites, seminars and educational visits to each other's facilities. These mutual projects mean that the departments meet and

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<sup>16</sup> The Technical Department handles questions about water supply, the sewage system and related issues. In some cities this service is outsourced and is not a direct part of the municipal organisation.

<sup>17</sup> The City Planning Department handles questions about building permits and city-planning.

get to know each other and thus clarify their roles in advance, which is very important as it facilitates organisation at the accident site.

As well as these local forms of cooperation, several EHPDs are also involved in regional committees or special groups, sometimes administered by the county administrative board, and sometimes through their own initiative. In a few cases such cooperation is mainly based on lessons learned from accidents in the region, but it often includes more general consideration of chemical phenomena, and in some cases training exercises related to chemical accidents are held.

Most EHPDs claim that their views are heard in other departments. Only one problem related to other departments was raised during the interviews: the conflict between exploitation and environmental concerns. For example, when a company wants to build a new plant at a new site they often believe that they can start building as soon as they get a building permit from the CPD, without checking with other authorities like the FRS or EHPD. This might lead to serious flaws related to human or environmental safety, and sometimes the building has to be stopped for such reasons. Such delays are due to a lack of communication between the CPD and the EHPD.

Nevertheless, most of the EHPDs have a positive attitude towards cooperation with other departments, and respect for them, especially the FRS, even though one EHO said “you have to work hard to ensure that your opinion is heard in the discussions”, they are becoming more open to cooperation and discussion than they were.

### *8.8 Further education, practical tools and lessons learned*

The general opinion of the EHPDs is that chemical accidents are not given a high priority. It is usually taken for granted that the organisation and knowledge of the officers will be sufficient to cope when an accident occurs, but when an accident happens the EHPDs also feel that they can take the time they need. Other opinions are that the personnel at the EHPD themselves can plan their schedules and hence, in theory, allocate time for further education and literature studies in the field. However, this time is often consumed by other, more urgent tasks.

Two subjects, geology (especially hydrogeology) and chemistry, were most commonly mentioned by the environmental officers at the EHPDs in discussions about the type of knowledge they felt they lacked or needed to

increase. Several officers would like to see more specialised courses focusing on these topics in relation to chemical accidents. Toxicology and risk analysis were other areas of concern for the officers.

To address these concerns, the officers were asked what they would wish for, if they could have any kind of tool or assistance to facilitate the handling of chemical accidents, regardless of costs. One of the most highly desired tools was a concise, simple handbook listing chemicals (and maybe groups of chemicals), together with information on their toxicity, how they are likely to spread in different environments and how to handle them. Ideally, therefore, they would like a diagnostic tool in which they could put in relevant chemical and environmental data and get a diagnosis of the situation together with the “medicine” to treat it. Other officers talked about handbooks for chemicals only, or for soils and their spreading properties. In addition, many officers would like to see a 24-hour expert centre to call about questions relating to chemicals, toxicity and environmental effects.

Another desired tool was a databank for lessons learned, in which contact details of relevant people and further references could be entered with each accident case. As a less time-consuming alternative, one environmental officer talked about building a simple network, which officers from all over the country could log onto and ask the others questions related to chemical accidents. Other desired tools included: extensive checklists and lists giving tolerance limits for different kinds of chemical spills (should there be a zero-tolerance limit?), computers with all the available information, environmental sensitivity maps, and practical exchange of lessons learned through large nationwide seminars once or twice a year.

### *8.9 The role of the responsible authorities*

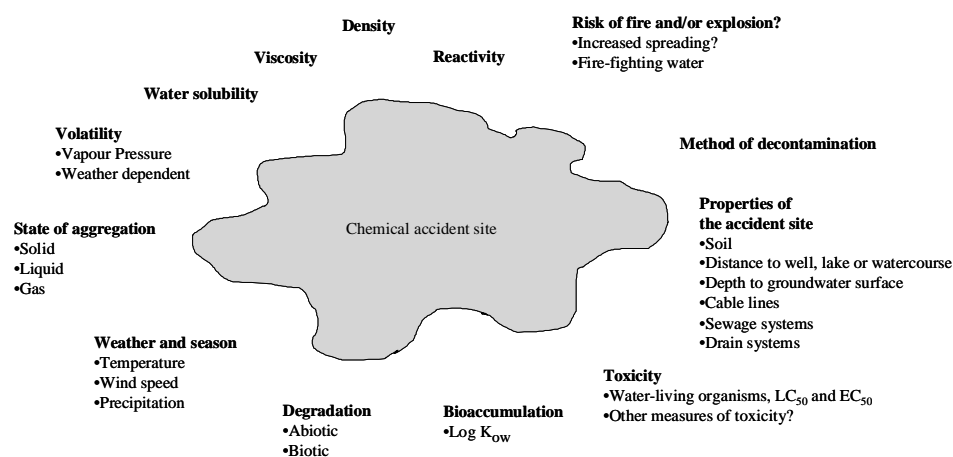
When the environmental officers were asked about their opinion of the responsible authorities; the Swedish Rescue Services Agency (SRSA), the Swedish Environmental Protection Agency (EPA) and the Swedish National Chemicals Inspectorate, they felt that most activity, help and support came from the Swedish National Chemicals Inspectorate and sometimes the SRSA, even though the SRSA is not the mother organisation of the EHPDs. The EPA (the mother organisation) was considered not to be pro-active in these respects (except for one municipality), and to offer little help.

## 9 Concluding remarks and future perspectives

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In this thesis several steps in the development of the EAI have been described. The work has yielded a lot of new knowledge and experience related to chemical accidents, but it has also raised many questions and suggestions for additional research.

The handling of a chemical accident is aimed to hinder the spread of the chemical, and to reduce its effects on the environment, human beings and property. This process requires the consideration of both chemical properties and properties of the accident site, as well as external factors like the weather and the type of decontamination method used. Figure 24 illustrates important factors to consider in this process.



**Figure 24.** Factors to consider at a chemical accident site.

While assembling data on the accidents I experienced many difficulties in accessing the information needed for the project. It should be noted that  $EAI_{new}$  only covers the accidents in the assembled dataset, and it is possible that more information on other chemical accidents could add useful knowledge for further development of the model. As chemical accidents cannot be designed, controlled or reproduced like common laboratory experiments, we have to handle information obtained from real-life accidents carefully. Undoubtedly, a lot of information about chemical accidents and experience related to them is available within the organisation(s) that handle them, both in Sweden and in other countries. However, most of this information is not gathered in such a way that others

can learn from it. I believe that we should learn not only from the large, severe accidents, but also from the more frequent, smaller accidents, which can also cause large effects in the environment (and are, therefore, equally important). This fact was also stressed during the interviews, where some suggestions were made on how to address this lack of communication, for instance the establishment of a simple e-mail network where people can easily ask questions and give links to sources of information. Another suggestion was to have large, nationwide seminars once or twice a year to present and discuss experience related to accidents. A more time consuming proposal is to build a new system for reporting chemical accidents from an environmental perspective, or to expand the system managed by the Swedish Rescue Services Agency, to also include environmental effects and fill their databank, RIB (*The Swedish Rescue Services Agency 2003*) with more information on lessons learned than it currently does. I realise that certain factors like limitations of resources and time conflict with these recommendations, but I still think that knowledge and experience from chemical accidents should be disseminated as widely as possible to prevent (or at least minimise) their adverse environmental consequences.

During the work on EAI the literature study was poorly rewarded, and only a few interesting models or indices were found. However, models may have been developed that have never been published in scientific journals and are therefore hard to find. The scarcity of published models also means that very few have been peer-reviewed, hindering the establishment of common ground for evaluation of the models. This seems to be a major, general problem within applied science, and it is important to break this trend since increasing the number of published articles in scientific journals would disseminate knowledge and facilitate cooperation, which in turn would accelerate the development of functional models.

The most crucial step in the development of the model so far was the selection of a representative set of accidents for use during the building of a new model. The aim was to establish a wide, unbiased but controlled basis for further development, in which the accidents were selected as representatives of a diverse set of accident scenarios. This approach is different from that used to develop other models/indices, (described in Chapter 1), which have been constructed for specific scenarios and afterwards applied to similar scenarios.

To develop a model like  $EAI_{new}$ , it is necessary to have a response describing the environmental impact of the accidents and to relate the calculated index to this impact. This was a difficult step as the responses

used at present are related to laboratory data on single effects in the environment and I wanted an overall estimation of several combined environmental effects. The decision to use experts to judge environmental effects was taken after the few alternative approaches had been discussed. The complexity of the environment, in combination with the very small amounts of research done in this field, made this an interesting approach.

However, working with human material was a new experience that required a different approach and a different way of thinking from those commonly used in natural science. Human material is difficult to handle, and the results showed that the expert judgements were not always unanimous, which is understandable. The question is: how wide-ranging can judgements of an accident be to remain acceptable and valid for different parts of Sweden? It is also possible that a lack of relevant knowledge, especially of hydrogeology, chemistry and limited experience of handling real chemical accidents (since they are relatively unusual), together with too narrow dissemination of information gained from experience, have contributed to the deviations. These hypotheses were corroborated during the interviews with the experts, some of whom made suggestions regarding the kind of additional help they would like from responsible authorities, such as the Swedish Environmental Protection Agency and the Swedish Rescue Services Agency, in order to improve their handling of chemical accidents. Their suggestions included provision of useful tools like databases and models such as the EAI, specific courses on appropriate topics and information centres that could be called at any time to answer questions on chemicals and their environmental effects.

The conclusions from the development of a new EAI model are that simple soil-related variables must be reconsidered. The development also showed that the added variables,  $P_v$  and  $D$  were relevant for the EAI approach. Further, it was shown that the chemical property variables ( $P_v$ ,  $D$  and  $S_w$ ) still have a stronger influence on the magnitude of the EAI than the site-specific properties ( $DNW$ ,  $DGS$  and  $SGS$ ), while  $m/Tox$  is and probably shall remain the most important variable. This means that the site-specific variables have to be given greater influence (larger weight).

The development process resulted in a new model,  $EAI_{new}$ .  $EAI_{new}$  is based on a set of data selected to represent a broader spectrum of chemical accident scenarios, so  $EAI_{new}$  has a better foundation than the other investigated models/indices.

$EAI_{new}$  can be calculated without the use of tables, and can estimate environmental effects, as well as make a rough classification of accidents according to the new classification scale.  $EAI_{new}$  can be re-expressed as a regression model based on the regression coefficients for one response at a time, in this thesis exemplified by response 2A. To facilitate the calculations even further, it would be easy to make lists of pre-calculated chemical properties together with data on the toxicity of the most frequently handled organic chemicals, so that only the site-specific properties and the amount of the chemical involved would have to be entered when assessing an accident. Such a model could allow people or authorities with scarce financial and personnel resources to estimate the environmental effects of chemical accidents as thoroughly as counterparts with more resources.

### 9.1 Future work

The work on  $EAI_{new}$  will continue and the highest priority issues should be:

- To validate  $EAI_{new}$  externally, to confirm its predictive power.
- To refine the structure of the formula through further consideration of:
  - $S_w$  – how should it be handled in the formula?
  - Soil variables – can simpler variables be used?
  - Weights of the variables, especially site-specific variables
- To further refine the classification scale, modifying the classes where necessary, developing more extensive recommendations, and perhaps checklists connected to each class regarding the way the results of the EAI calculation should be treated.
- A real-life validation in which  $EAI_{new}$  is tested by people working with chemical accidents.
- Toxicity: as the toxicity is the most important variable in the formula, other measures of toxicity should be considered. The use of cells exposed to the bio-available fraction of a chemical as discussed in Chapter 2.4 might provide a useful measure of toxicity, representing the toxicity to soil-living organisms.

Other issues of interest in a longer term perspective might include the construction of EAI:s for other applications, and an EAI for inorganic chemicals. Other refinements could include EAI:s for fire scenarios, gases,

response-specific (terrestrial and aquatic) and season-dependent (weather and temperature) indices. The fact that  $EAI_{new}$  is currently restricted to organic chemicals and the specified responses does not mean that other chemicals, responses or other scenarios will be excluded forever. The only limiting factors might be the costs, in terms of both resources and time, of such projects.

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A handwritten signature in black ink, appearing to be the name 'Mira' with a small decorative flourish at the end.

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## Appendix I

**Table 1.** Distance to nearest well, lake or watercourse.

|                |      |       |       |       |         |          |           |            |             |        |
|----------------|------|-------|-------|-------|---------|----------|-----------|------------|-------------|--------|
| <b>Value:</b>  | 9    | 8     | 7     | 6     | 5       | 4        | 3         | 2          | 1           | 0      |
| <b>Meters:</b> | 0-10 | 10-20 | 20-35 | 35-50 | 50 - 75 | 75 - 150 | 150 - 300 | 300 - 1000 | 1000 - 2000 | > 2000 |

**Table 2.** Depth to groundwater surface.

|                |         |         |     |     |     |      |       |         |         |      |
|----------------|---------|---------|-----|-----|-----|------|-------|---------|---------|------|
| <b>Value:</b>  | 9       | 8       | 7   | 6   | 5   | 4    | 3     | 2       | 1       | 0    |
| <b>Meters:</b> | 0 - 0.2 | 0.2 - 1 | 1-3 | 3-5 | 5-7 | 7-12 | 12-20 | 20 - 30 | 30 - 60 | > 60 |

**Table 3.** The leaning of the groundwater surface and the flow direction

|               |   |                                       |   |
|---------------|---|---------------------------------------|---|
| <b>Value:</b> | 5   | 1                                     | 0   |
|               | Groundwater surface is inclined towards a well, lake or watercourse | The groundwater surface is horizontal | No well, lake or watercourse is laying within 1 km of the direction of the groundwater flow |

**Table 4.**

Choose the lowest point in the interval if the rock beneath the soil is massive.

| The thickness of the soil | Value: |      |         |      |      |                |
|---------------------------|--------|------|---------|------|------|----------------|
|                           | Gravel | Sand | Moraine | Silt | Clay | Frosted ground |
| > 30 m                    | 9      | 8    | 6       | 4    | 0    | 0              |
| 25 - 30                   | 9      | 7-8  | 5-6     | 3-5  | 0-1  | 0              |
| 20 - 25                   | 9      | 7-8  | 5-6     | 3-5  | 0-2  | 0              |
| 15 - 20                   | 9      | 7-8  | 5-7     | 3-6  | 0-3  | 0              |
| 10-15                     | 9      | 7-9  | 5-8     | 3-7  | 0-4  | 0              |
| 3-10                      | 9      | 7-9  | 6-8     | 4-8  | 1-6  | 0              |
| < 3                       | 9      | 7-9  | 6-9     | 4-8  | 2-8  | 0              |

# Appendix I

**Table 5.** Values for the variable Sur

| Summarized values from Tables 1-4 | Value (Sur) |
|-----------------------------------|-------------|
| >25                               | 10          |
| 20-25                             | 7           |
| 15-20                             | 5           |
| 10-15                             | 3           |
| <10                               | 1           |

**Table 6.** Values for the variable Tox

| Acute toxicity <sup>a</sup><br>(LC <sub>50</sub> or EC <sub>50</sub> ) mg/L | Value (Tox) |
|---|-------------|
| <1 <sup>b</sup>   | 10          |
| 1-6   | 8           |
| 6-30  | 6           |
| 30-200  | 4           |
| 200-1000  | 2           |
| >1000   | 1           |

a) Use the lowest available LC<sub>50</sub>-value or EC<sub>50</sub>-value for fish, *Daphnia* or algae.

b) Handling of extreme toxic chemicals should be investigated even if the calculated EAI-value will be low.

**Table 7.** Values for the variable Con

| Consistency<br>Viscosity <sup>a</sup> (cSt) <sup>b</sup> | Value (Con) |
|--|-------------|
| <0.5   | 5           |
| 0.5-4.4  | 4           |
| 4.4-47   | 3           |
| 47-300   | 2           |
| >300   | 1           |
| Solid compound   | 0           |
| Unknown viscosity  | 4           |

a) If data about the viscosity is missing use value 4 that correspond to the viscosity interval where most liquid chemicals can be found.

b) If the viscosity only is available as cp (centipois) this value is first divided with the density of the chemical in g/cm<sup>3</sup>

**Table 8.** Values for the variable Am

| Stored or transported amount of the chemical (metric tonnes) <sup>a</sup> | Value (Am) |
|---|------------|
| >500 <sup>b</sup>   | 10         |
| 50-500  | 7          |
| 5-49  | 5          |
| 0.5-4.9   | 3          |
| <0.5  | 1          |

a) The maximal amount of the chemical, converted into pure compound, that can be handled

b) Extreme large stocks should be investigated even if the calculated EAI-value will be low.

**Table 9.** Values for the variable Sol

| Water solubility (weight-%) | Value (Sol) |
|-----------------------------|-------------|
| >90                         | 5           |
| 25-90                       | 4           |
| 5-25                        | 3           |
| 1-5                         | 2           |
| <1                          | 1           |
| Solved in water             | 5           |
| Solved in organic solvent   | a           |

a) The solubility value for the solvent

## THEORETICAL SENSITIVITY TEST

The test aimed to analyse the different parameters in the formula to study their individual importance for the magnitude of the EAI. The procedure is exemplified below by a test of the variable **Sol**.

Calculation of EAI when the parameter **Sol** (water solubility) is varied and the other parameters in the formula have a fixed value. In cases where a chemical matching one value level is missing, a fictive chemical is used, for example “Chem A”.

The chemicals used in this test are:

Copper Sulphate (l) and(s)  
Aniline  
ortho- Xylene  
Potassium Cyanide (s)  
DDT (s)  
Some fictitious chemicals

The chemicals are given a value according to tables 6-9, which depends on their properties. The parameters **Am** and **Sur** are given the value 5 respectively to simulate a “normal situation”.

$$EAI_{(o\text{-Xylene})} = 10 \times 5 \times (4+1+5) = 500$$

$$EAI_{(\text{ChemA})} = 10 \times 5 \times (4+2+5) = 550$$

$$EAI_{(\text{ChemB})} = 10 \times 5 \times (4+3+5) = 600$$

$$EAI_{(\text{Aniline})} = 10 \times 5 \times (4+4+5) = 650$$

$$EAI_{(o\text{-Xylene})} = 10 \times 5 \times (4+5+5) = 700$$

|                  |                 |                 |
|------------------|-----------------|-----------------|
| <b>CuSO4(l):</b> | <b>“ChemA”:</b> | <b>“ChemB”:</b> |
| Tox=10           | Tox=10          | Tox=10          |
| Con=4            | Con=4           | Con=4           |
| Sol=5            | Sol=4           | Sol=3           |

|                 |                  |
|-----------------|------------------|
| <b>Aniline:</b> | <b>o-Xylene:</b> |
| Tox=10          | Tox=10           |
| Con=4           | Con=4            |
| Sol=2           | Sol=1            |

$$EAI_{(\text{DDT})} = 10 \times 5 \times (0+1+5) = 300$$

$$EAI_{(\text{ChemA})} = 10 \times 5 \times (0+2+5) = 350$$

$$EAI_{(\text{CuSO4})} = 10 \times 5 \times (0+3+5) = 400$$

$$EAI_{(\text{KCN})} = 10 \times 5 \times (0+4+5) = 450$$

$$EAI_{(\text{ChemB})} = 10 \times 5 \times (0+5+5) = 500$$

|             |                 |                  |
|-------------|-----------------|------------------|
| <b>DDT:</b> | <b>“ChemA”:</b> | <b>CuSO4(s):</b> |
| Tox=10      | Tox=10          | Tox=10           |
| Con=0       | Con=0           | Con=0            |
| Sol=1       | Sol=2           | Sol=3            |

|             |                 |
|-------------|-----------------|
| <b>KCN:</b> | <b>“ChemB”:</b> |
| Tox=10      | Tox=10          |
| Con=0       | Con=0           |
| Sol=4       | Sol=5           |

## Appendix III

### Calculation of EAI for 49 different chemicals

In part two of the theoretical evaluation the original EAI was calculated for 49 different chemicals during the variation of the parameters Am and Sur. The parameters Am and Sur can each get five different value levels (10,7,5,3 and 1 point according to table 5 and 8 in Appendix I) and this leads to 25 different combinations during the calculations. 25 different combinations of the parameters Am and Sur for 49 different chemicals gives 1225 permutations. The result of the calculations is summarized below. The summary shows the distribution of the calculated EAI values (in %) to the different risk categories.

| Values for Am and Sur: | Riskcategories: |            |            |
|------------------------|-----------------|------------|------------|
|                        | 0 - 100         | 100 - 500  | >500       |
| Am = 1 Sur = 1         | 46              | 3          | 0          |
| Am = 3 Sur = 1         | 20              | 29         | 0          |
| Am = 5 Sur = 1         | 15              | 31         | 3          |
| Am = 7 Sur = 1         | 15              | 29         | 5          |
| Am = 10 Sur = 1        | 6               | 31         | 12         |
| Am = 1 Sur = 3         | 46              | 3          | 0          |
| Am = 3 Sur = 3         | 17              | 32         | 0          |
| Am = 5 Sur = 3         | 12              | 34         | 3          |
| Am = 7 Sur = 3         | 12              | 28         | 9          |
| Am = 10 Sur = 3        | 2               | 27         | 20         |
| Am = 1 Sur = 5         | 41              | 8          | 0          |
| Am = 3 Sur = 5         | 15              | 34         | 0          |
| Am = 5 Sur = 5         | 12              | 29         | 8          |
| Am = 7 Sur = 5         | 11              | 19         | 19         |
| Am = 10 Sur = 5        | 2               | 16         | 31         |
| Am = 1 Sur = 7         | 38              | 11         | 0          |
| Am = 3 Sur = 7         | 13              | 36         | 0          |
| Am = 5 Sur = 7         | 12              | 26         | 11         |
| Am = 7 Sur = 7         | 3               | 23         | 23         |
| Am = 10 Sur = 7        | 0               | 17         | 32         |
| Am = 1 Sur = 10        | 28              | 21         | 0          |
| Am = 3 Sur = 10        | 12              | 34         | 3          |
| Am = 5 Sur = 10        | 11              | 17         | 21         |
| Am = 7 Sur = 10        | 2               | 16         | 31         |
| Am = 10 Sur = 10       | 0               | 15         | 34         |
| <b>Sum:</b>            | <b>391</b>      | <b>569</b> | <b>265</b> |
| <b>% of total:</b>     | <b>32</b>       | <b>46</b>  | <b>22</b>  |