Site characterization and risk assessment of organic groundwater contaminants in South Africa

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THESIS
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Abstract

South Africa has only recently realized that organic groundwater contamination occurs in this country and that it can have a serious effect on the groundwater quality. The Water Research Commission (WRC) recently launched studies to investigate Non Aqueous Phase Liquid (NAPL) pollution, and Dense NAPL in specific. The understanding of NAPL pollution problems, is however, still very limited. Hence groundwater practitioners confronted with NAPL pollution problems have burning questions regarding amongst others the characterization of the pollution, which is much more sophisticated than in the case of inorganic pollution. While in this phase, groundwater practitioners can not even begin to consider remedial efforts for contaminated sites, which continue to pollute the groundwater. It is therefore of paramount importance to get up to speed with technologies and practices accepted worldwide for characterization. Much improvement is still needed on these characterization methods, but South Africa can learn from past mistakes made by other countries in addressing NAPL pollution.

In order to begin contemplating addressing NAPL characterization, it is important to understand the nature of the problem, which is why Chapter 2 describes the current situation of organic groundwater pollution and the associated vulnerability of aquifers in South Africa. The general understanding of groundwater pollution by NAPL is distorted, not only in the eyes of the public, but also in the eyes of experts in the groundwater field. A general misconception is that NAPL pollution only occurs at heavy industries such as ISCOR and SASOL, but Chapter 2 clearly shows that organic pollution is much more widespread and sinister in nature than would have been thought before. Smaller urban activities and small industries have been identified to be just as large a contributor towards organic pollution as the heavy industries. Shortcomings in the current understanding of NAPL pollution have been highlighted in Chapter 2 and further studies can be focused on determining the current impact of various industries on groundwater in South Africa, as well as delineating towns in which leaking underground storage tanks may be a problem. In order to address the NAPL pollution problem, legislative tools have to be in place. Gaps in legislation have therefore also been highlighted, of which several are listed in Chapter 3. These concerns need to be addressed by making the applicable policies and regulations, and implementing these regulations. In order to shed light on how site assessment and characterization can be performed in South Africa, Chapters 4, 5, 6 and 7 address issues associated with site assessment and characterization. Risk assessment has also been addressed (Chapter 8) and several shortcomings, to be addressed by toxicologists and groundwater practitioners, have been highlighted.

It was clear from the investigations performed throughout this thesis, that several shortcomings exist in association with site assessment, site characterization and risk assessment, which will need to be addressed in the near future.

Keywords: Industries, South Africa, organic pollution, vulnerability, NAPL, site assessment, site characterization, impact assessment, risk assessment.

Uittreksel

Suid Afrika het eers onlangs besef dat organiese grondwater besoedeling in die land voorkom en dat dit ‘n groot effek op die grondwater kwaliteit kan hê. Die waternavorsings kommissie (WNK) het onlangs ondersoeke geloods na organiese besoedeling, en spesifiek swaar olie besoedeling. Die vlak van kennis van organiese besoedeling is egter nogsteeds baie laag. Grondwater kundiges het dus brandende vrae aangaande byvoorbeeld die karakterisering van organiese grondwater besoedeling, wat soms meer gespesialiseerd is as in die geval van anorganiese besoedeling. Dit is dus van kardinale belang dat Suid-Afrika homself verwitting van internasionale standaard en praktyk in terme van die aanspreek van organiese grondwater besoedeling. Die internasionale gemeenskap kan nog baie verbetering aanbring op die terrein van karakterisering, maar Suid-Afrika kan baie uit die foute van ander lande in hulle pogings om organiese grondwater besoedeling aan te spreek, leer.

In ‘n poging om die karakterisering van organiese grondwater besoedeling te verstaan, is dit nodig om die omvang van organiese besoedeling in Suid-Afrika te verstaan. Dit word in Hoofstuk 2 beskryf. Die hoofstuk spreek ook die kwesbaarheid van grondwater vir organiese besoedeling aan. Die publiek en grondwater kundiges het oor die algemeen ‘n wanopvatting van organiese grondwater besoedeling in Suid-Afrika, waarvan een die opvatting is dat organiese grondwater besoedeling net by swaar industrieë soos byvoorbeeld ISCOR en SASOL voorkom, maar Hoofstuk 2 lig dit duidelik uit dat organiese grondwater besoedeling baie meer algemeen en en van groter omvang is as wat voorheen gemeen is. Die afleiding is gemaak dat kleiner industrieë en klein stedelike aktiwiteite net so ‘n groot bydrae kan lewer tot organiese grondwater besoedeling as swaar industrieë. Tekortkominge in die huidige vlak van kennis van organiese grondwater besoedeling is in Hoofstuk 2 uitgelig en verdere studies kan daarop fokus om die impak van verskillende industrieë op organiese besoedeling van grondwater te identifiseer. Dorpe wat brandstoftenks het wat lek, moet geïdentifiseer word. Wette moet in plek gestel word om die besoedelingsprobleem aan te spreek. Dit word aangespreek in Hoofstuk 3, waar daar aanbeveel word om regulasies af te kondig wat organiese grondwater effektief aanspreek. Hoofstukke 4, 5, 6 en 7 spreek die vraagstuk van die assessering van organiese besoedeling en die karakterisering van besoedelingsterreine aan. Risikobepaling word in Hoofstuk 8 aangespreek en tekortkominge wat deur toksikoloë en grondwater kundiges aangespreek moet word, is geïdentifiseer.

Dit was duidelik vanuit die ondersoeke wat in die tesis aangepak is, dat daar heelwat tekortkominge in die velde van asessering en karakterisering van organiese grondwater besoedeling bestaan, wat in die nabye toekoms ernstig aangespreek sal moet word.

Sleutelwoorde: Industrieë, Suid-Afrika, organiese besoedeling, grondwater kwesbaarheid, olies, terrein assessering, terrein karakterisering, impakstudies, risikobepaling.

Table of contents

CHAPTER 1: INTRODUCTION

CHAPTER 2: ORGANIC POLLUTION IN SOUTH AFRICA

CHAPTER 3: LEGISLATION

CHAPTER 4: NAPL PHYSICAL PROPERTIES AND OTHER PARAMETERS REQUIRED

CHAPTER 5: NAPL SITE ASSESSMENT

CHAPTER 6: SITE CHARACTERIZATION

CHAPTER 7: IMPACT ASSESSMENT

CHAPTER 8: RISK ASSESSMENT

CHAPTER 9: SUMMARY

CHAPTER 10: REFERENCES

APPENDICES:

List of figures

CHAPTER 2: ORGANIC POLLUTION IN SOUTH AFRICA

CHAPTER 3: LEGISLATION

CHAPTER 4: NAPL PHYSICAL PROPERTIES AND OTHER PARAMETERS REQUIRED

CHAPTER 5: NAPL SITE ASSESSMENT

CHAPTER 6: SITE CHARACTERIZATION

CHAPTER 7: IMPACT ASSESSMENT

CHAPTER 8: RISK ASSESSMENT

List of tables

CHAPTER 2: ORGANIC POLLUTION IN SOUTH AFRICA

CHAPTER 4: NAPL PHYSICAL PROPERTIES AND OTHER PARAMETERS REQUIRED

CHAPTER 5: NAPL SITE ASSESSMENT

CHAPTER 6: SITE CHARACTERIZATION

CHAPTER 7: IMPACT ASSESSMENT

CHAPTER 8: RISK ASSESSMENT

Chapter 1

Introduction

Non-**A**queous **p**hase **l**iquids (NAPLs) are immiscible fluids with a density other than that of water. Numerous contamination sites exist in South Africa and the problem has only recently received attention where NAPL research in the United States of America and Europe has been underway for a few years now.

The subsurface movement of NAPL is controlled substantially by the nature of the release, the NAPL density, interfacial tension, viscosity, porous media capillary properties and to a lesser extent hydraulic properties. Visual detection of NAPL in soil and groundwater samples may be difficult where the NAPL is transparent, present in low saturation or distributed heterogeneously. These factors confound characterization of the movement and distribution of the NAPL. Fractured bedrock, heterogeneous strata and multiple NAPL mixtures further compound the difficulty of site characterisation.

Obtaining a detailed delineation of subsurface NAPL can therefore be very costly and it may be impractical using conventional site investigation techniques. The risk of causing NAPL migration by drilling or other actions may be substantial and should be considered prior to commencing fieldwork. NAPL can greatly complicate site characterization but failure to adequately define its presence, fate and transport can result in misguided investigation and remedial efforts. Large savings and environmental benefits can be realized by conducting site investigation studies in a cost-effective manner.

1.1 SCOPE OF THE STUDY

The scope of the investigation is as follows:

1. To describe the current situation of organic groundwater pollution in South Africa. The aim is to determine the types of waste streams and volumes produced in South Africa by various industries. The selected industries will be plotted for South Africa in order to form an idea of intensity and spatial distribution of the industries. These industries will also be plotted on an aquifer vulnerability map in order to identify industrial aquifer vulnerable areas. From this information towns with possible organic pollution will be identified, and research needs will be identified.

2. Detailed descriptions of NAPL migration, the legislative background and shortcomings in the regulations, as well as methods for detection and testing of NAPLs in South Africa will be given.

3. An evaluation of site characterization and risk assessment of organic contaminants in South Africa is performed, giving guidance to the improvement thereof. Different risk assessment methods will be compared in order to determine the applicability and use of several risk assessment methods (e.g. the Environment Agency's R&D approach and the RISC Workbench Model, as well as the URA developed by the Institute for Groundwater Studies (IGS).

1.2 THE STRUCTURE OF THE THESIS

1. Organic groundwater contamination will be described in Chapter 2, while the South African legislation has been investigated in Chapter 3. It is attempted to point out gaps in current legislation and proposing regulations in order to enhance the effectiveness of the legislation. International law has also been reviewed and NAPL related treaties that could aid South Africa in handling the NAPL pollution problem are highlighted.

2. The parameters that laboratories in South Africa are able to determine will be listed in Chapter 4, as well as laboratory prices for parameter estimation. The shortcomings of the labs in South Africa and areas in which the labs can be upgraded will then be listed. An Appendix on organic parameters (textbook values) is given for chapter 4, which will be used again in Chapter 7 for the calculation of certain parameters. This info will also be used in Chapter 8 (Risk assessment) for the risk example calculations. A review of site characterization methods will be given (Chapter 6), to which the applicability in hard rock areas will be highlighted. The use of the methods for NAPL delineation will also be highlighted.

3. A case study will be presented in which site assessment (Chapter 7); site characterization (Chapter 7) and risk assessment (Chapter 8) will be performed. With this it will be aimed to highlight shortcomings in current methodologies and the input data for the risk assessment models.

Chapter 2

Organic groundwater pollution in South Africa

2.1 INTRODUCTION

The aim of this chapter is to list industries that are associated with organic pollution (Section 2.1.4), list the organic chemicals associated with industrial groundwater pollution (Section 2.1.6.1), and generate an industrial aquifer vulnerability map specifically for organic groundwater contamination in South Africa. Background information will be given on the chemical industries history (Section 2.1.1) and the general process of chemical industries (Section 2.1.3). In Section 2.1.5 the volumes of chemicals produced annually in South Africa are given. All the above-mentioned information aid in understanding organic chemicals and the associated pollution and risk. In Section 2.1.7 the data from Section 2.1.6.1 and data from STATS SA, as well as aquifer vulnerability maps, are combined to generate industrial maps (Section 2.1.7.3) and lastly an industrial aquifer vulnerability map (Section 2.2).

2.1.1 The History

General industrialization began in the early 1880's with the discovery of gold in the mid-1880's (Lumby, 1995). The first iron and steel plant (ISCOR) was opened at Pretoria West in 1934 (Cross, 1994). During the Second World War (1945) provided a spur in the iron, steel and engineering sectors (Lumby, 1995). ISCOR's production capacity increased from 300 000 tonnes before the war to 450 000 tonnes by 1945. This increase enabled South Africa to produce roughly half of its steel requirements (Cross, 1994).

The chemicals industry in South Africa was founded in the latter part of the nineteenth century as a result of the demand for explosives and chemicals to support the mining industry (Mbendi, 2003), while the establishment of a petrochemicals industry can be traced back to the 1950's (Giantsos, 1995). Two large synthetic oil-from-coal plants by Sasol at Secunda were established during the early 1980's to provide strategic self-sufficiency in fuels. The synfuel sector, while serving the South African oil industry as a source of fuels, is now also the major source of chemical feedstocks and intermediates in South Africa (Mbendi, 2003). A plant for polyvinyl chloride (PVC) was established in 1955, and plants for polyethylene in 1966, polystyrene in 1964, synthetic rubbers in 1964 and latex in 1968 (Giantsos, 1995). Giantsos (1995) observed that the demand for output from the petrochemical industry is widely dispersed across various sectors of the economy. This can be seen in Section 2.1.4 where industries employing organics (and are thus related to the petrochemical industry) are listed.

2.1.2 Industry Structure

South Africa's chemical industry is of substantial economic significance to the country, contributing around 5% to GDP and approximately 25% of its manufacturing sales. (DEAT (a), 2003) The industry is highly complex and widely diversified, with end products often being composed of a number of chemicals, which have been combined in some way to provide the required properties and characteristics. Annual production of primary and secondary process chemicals is in the order of 13 million tonnes with a value around 18 billion Rand (1.5 billion US$). (CAIA, 2002)

2.1.2.1 Categorization of chemicals

The different chemicals produced, can be divided into four broad categories (DEAT (a), 2003):

- Base chemicals
- Intermediate chemicals
- Chemical end-products
- Speciality end-products

Base chemicals including ethylene, propylene, butadiene, benzene, toluene, xylenes, and methanol are all important petrochemical building blocks sourced from the petrochemical industry. Inorganic base chemicals are amongst others the following: ammonia, caustic soda, sulphuric acid, chlorine, sulphur and soda ash (Mbendi, 2003). The primary products 1 and 2 in the flow chart in Section 2.1.3 represent the base chemicals.

Using the Fischer Tropsch process, Sasol produces about two million tonnes per annum of a range of various olefins for the petrochemical industry. About 0.6 million tonnes of olefins are used by the chemical industry, and the remaining 1.4 million tonnes is used in fuels. A small proportion (about 25,000 tonnes) is recovered from crude oil refineries. The Engen refinery in Durban produces some benzene and other aromatics. Modest amounts of propylene are produced at the Sapref refinery in Durban. The Mosref plant generates mixed alcohol and ketone streams, which are currently exported. According to DEAT (a) (2003) Sasol is the largest single producer of primary chemicals.

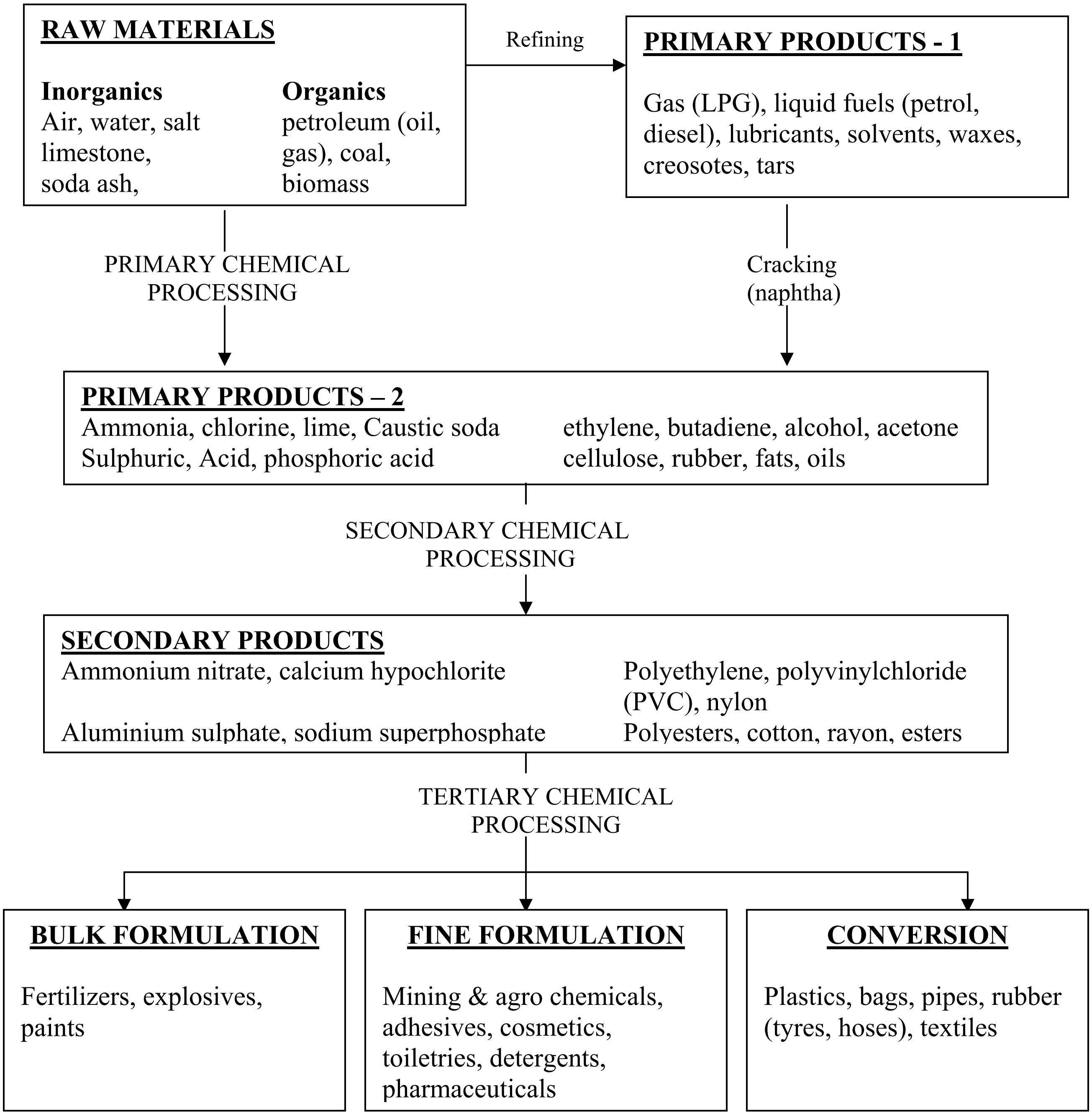
Intermediate chemicals is a term which can be used to describe a plethora of products such as ammonia, waxes, solvents, phenols, tars, plastics, and rubbers. Major organic secondary products include polyethylene, polypropylene, polyvinyl chloride as well as nylon, polyester and acrylic fibers. The secondary products in the flow chart in section 2.1.3 represent the intermediate chemicals.

Chemical end products include processible plastics, paints, explosives, and fertilisers. The bulk formulation and conversion products in the flow chart in section 2.1.3 represent the intermediate chemicals.

Specialty chemical end products are lower volume, higher added-value chemical products. Chemicals like pharmaceuticals, agro-chemicals, bio-chemicals, food-, fuel- and plastics - additives fall into this category. The fine formulation products in the flow chart in section 2.1.3 represent the intermediate chemicals.

2.1.3 General Process of Chemical Industries

The following general model of Chemical Industries has been obtained from DEAT (a) (2003) and puts the production of the different categories of chemicals into perspective. These categories of chemicals are described in section 2.1.2.1.



2.1.4 Industries employing organic chemicals in the production of their products

Table 2-1 lists and describes chemical industrial processes in brief, to outline the role organic chemicals play in certain industries. The information in this section will be the basis of the industries chosen for the statistics given in Section 2.1.5, and for choosing the industries that have to be plotted on maps to create the industrial vulnerability map.

TABLE 2-1: Industries using organic chemicals

Industry	Chemicals employed, associated wastes
Explosives industry	Waste may include explosives components, such as di- and tri-nitro compounds, solvents (e.g. toluene, formaldehyde), and fuels (gasoline, diesel and aircraft fuels). (EPA, 2003 (a))
Paint industry	Little waste is generated by paint manufacturers, most of the materials are used up in the process. Waste products: volatile organic compounds, spent polymers, surfactants, anti-bacterial agents and mild corrosives (for cleaning the process line). Most of these compounds are in the form of sludges and/or solids and will harden over time if not utilized. These materials may be in drums, tanks or in the process lines themselves (EPA, 2003 (b)).
Manufacturing of ink, printing industry	Printing inks consist of pigments or dyes in a carrier (which may be a drying oil with or without natural or synthetic resins). The four top toxic chemicals released by the printing industries are (GLRPPR, 2003): Toluene (70% in total of toxic chemicals released), Methyl Ethyl Ketone (MEK), Xylene and 1,1,1-trichloroethylene
Tanning of animal skins	Polluting agents from animal products processing are 1) High organic matter concentrations (i.e. fats, oils, proteins, and carbohydrates); 2) High insoluble organic and inorganic particle content; and 3) the release of toxic compounds. (LEAD, 2003)
Production of pesticides	Waste products are often containerized on site in medium to large quantities for recycling into the process or disposal. Common organic waste products encountered include unused raw materials e.g. benzene, carbon tetrachloride and xylene (EPA, 2003 (c)).
Production of herbicides	There are several chemical antecedents shared by most of the herbicides used today. Their roots are in acetic acid, ammonia and coal tar. (Iowa State University Agronomy, 2003)
Production of perfumes, ointments and oils	These products contain organics as the carrier base for the aromatics. **Acetone** is found in cologne, dishwashing liquid & nail enamel remover. **Benzyl alcohol** is found in shampoo, laundry bleach, deodorants & fabric softener. **Ethanol** is found in hairspray, shaving cream, soap, air fresheners, paint & varnish remover. **Ethyl acetate** is found in after-shave, fabric softener & dishwashing liquid.
Food processing industries	Edible oil industries generate mostly oils & grease, which is the parameter used to measure wastewater generated by refining units and hydrogenated oil units – (e.g. industries refining oils from seeds and industries processing oils to soap (SEAM, 2003).

TABLE 2-1: Industries using organic chemicals (*contd.*)

Industry	Chemicals employed, associated wastes
Soap industry	Detergents, soap and glycerin are produced in the soap industry. The main organic effluent source in this industry consists of un-reacted fatty matter and glycerol (Mail Archive, 2003).
Fermentation industries	Industrial alcohol (ethyl alcohol) is produced for industrial use as solvent and for synthesis of other chemicals, beers, wines and liquor are produced for consumption. The main waste product from distilleries is organic waste in the form of used barley or wheat and large quantities of water containing organic chemicals. (Brink and Shreve, 1977)
Steel industry	Steel production involves three basic steps. 1) The heat source used to melt iron ore is produced. 2) The iron ore is melted in a furnace. 3) The molten iron is processed to produce steel. Organic wastes (oil and grease) are produced from pre-processing of feed materials, sinter and pellet plants and Coke ovens. (Brink and Shreve, 1977)
Pulp and paper industries	82% of pulping is carried out by chemical means. Kraft or sulfate pulp is a process used to remove the large amount of oils and resins in coniferous woods. The process involves cooking white liquor (caustic soda and sodium sulfate) which is added to wood chips while live steam is turned on. The spent cooking liquor (black liquor) is pumped to storage to await recovery of its chemicals by evaporation, where the dissolved organic material is usually combusted. The storage of black liquor may cause groundwater pollution problems if stored in unlined dams.
Plastic industry	Production of various plastics includes a series of organic processes using mainly petrochemicals. (Brink and Shreve, 1977)
Rubber industry	Rubber is produced either by collection of natural rubber or the synthesis of rubber using petrochemicals. Several organic chemicals are used as rubber processing chemicals – age restrictors (N-phenyl-2-napthylamine), softeners (petroleum oils, coal tar fractions), waxes (petroleum waxes), blowing agents (fluorocarbons) and chemical plasticizers (2-naphtalenethiol).
Petroleum refining	Various distillate products are derived from crude oil. These distillate products are processed to form the following products: Liquified petroleum gas, motor and aviation gasolines, kerosene, furnace oil, diesel oil, heavy fuel oils, asphalts, light and heavy lubricating oils and refined waxes. (Brink and Shreve, 1977)
Pharmaceutical industry	The pharmaceutical industry employs more complicated manufacturing processes than almost any other chemical industry and usually uses cyclic organic chemicals. Several processes exist for the production of pharmaceuticals, e.g. esterification (alcoholysis), methylation and complex chemical conversions. (Brink and Shreve, 1977)
Intermediates and dyes	The dye industry draws upon every division of the chemical industry for the multiplicity of raw materials needed to make the dyes. The main raw-material sequence, can, however, be presented as follows: Petroleum and coal→hydrocarbons → intermediates → dyes (Brink and Shreve, 1977).

2.1.5. Volumes of organic related products produced annually in South Africa

Information on products produced by industry in South Africa, has been obtained from Statistics SA.

Those pertaining to possible organic waste generation are listed below:

- Tanning extract
- Industrial chemicals (gases and organic compounds)
- Organic fertilizers (phosphatic fertilizers)
- Other fertilizers
- Organic insecticides (organophosphates)
- Other insecticides
- Herbicides
- Paints, varnishes, lacquers
- **Household:**
    - Candles
    - Creams
    - Bath oil and additives
    - Polishes
- **Petroleum products:**
    - Motor spirits
    - Aviation spirit
    - Fuel oil
    - Lubricating and process oils
    - Miscellaneous from petrol and coal (fuel gas)
- **Plastics:**
    - Plastic (primary forms – condensation and polymerization products)
    - Tyres and tubes
    - Not classified
    - Flooring and building material
    - Bags and sacks
    - Gutters and downpipes
    - Containers (Sasol: pvc, polypropylene, polyethylene)
    - Textile fabrics
    - Gardening and agricultural pipes
    - Packaging sheets and rolls

Volumes of organic products produced annually in South Africa:

The specific gravity (SG) of products produced by industry is important to convert the volumes of fluid chemicals to mass units, so as to be able to compare the production of different chemicals. Specific gravity is dimensionless unit, which is defined as the ratio of density of the material to the density of water at a specified temperature (Engineering Toolbox, 2003). It is also used to determine whether the NAPL is a sinker or floater, and can as such also be used to divide the different fluid chemicals into Light Non –Aqueous Phase Liquids (LNAPLs) and Dense Non-Aqueous Phase Liquids (DNAPLs).

Rules of thumb for the SG's of chemical products (e.g. paints) are:

- If the product is pigmented, the SG will have a very good chance of being over 1.
- If the product is clear, the SG will generally be less than 1.
- Coatings with organic pigments (some reds, blues and greens) and carbon black can be less than 1. (Personal communication: L Fischer, 2003)

In **TABLE 2-2**, production volumes for organic related chemicals in South Africa can be seen. SG values were only reported where they were necessary in order to convert a product from litres to kilograms and then to tonnages. Customs and Excise export and import figures were included in an attempt to make the figures of organic related chemical products residing in South Africa annually, more reliable. Large volumes of organics (especially petroleum and petroleum related products) are imported annually into South Africa.

Average SG's for the various products were estimated using various information sources and material safety data sheets obtained from companies such as Sasol and other international industries' product Material Safety Data Sheets (MSDS's). The SG's are referenced in **TABLE 2-2**. Some SG's could not be obtained or estimated since either the reported product grouping (insecticides and herbicides) or the grouping itself (cosmetics and toiletries) was too variable.

Usually volumes for 2002 were used, but where no statistics exist, volumes produced in previous years, were used as a substitute. The values are similar but will not precisely reflect the true figure of all volumes produced in the year 2002. A slight increase has been observed in most of the product's production for each successive year, thus the figure might be a slight under-estimate of the true volume.

TABLE 2-2: Production volumes for organic related chemicals in South Africa

STATS SA P3051.3 Feb 2003					**STATS SA P3051.3 Feb 2002 (DEAT (a), 2003)**	**SARS Customs & Excise (DEAT (a), 2003)**	
						Import	**Export**
Product	**Liters**	**SG**	**Kilograms**	**Tonnes**	**Tonnes**	**Tonnes**	**Tonnes**
Tanning extract	Reported in tonnes	Not Applicable (N/A)	N/A	53,826	Not Reported (N/R)	N/R	N/R
Industrial chemicals – organic	Reported in tonnes	N/A	N/A	909,608	861,000	641,000	1,211,000
Plastic – Primary Forms	Reported in tonnes	N/A	N/A	829,384	793,000	427,000	458,000
Fertilizers							
Phosphatic fertilizers	Reported in tonnes	N/A	N/A	369,000	N/R	N/R	N/R
Other fertilizers	Reported in tonnes	N/A	N/A	1,095,000	N/R	N/R	N/R
Total Fertilizers	Reported in tonnes	N/A	N/A	*1,464,000*	1,634,000	807,000	739,000
Insecticides – organo phosphates	4297000	Product Grouping too variable			N/R	N/R	N/R
Insecticides – Other	5792000	Product Grouping too variable			N/R	N/R	N/R
Incesticides – solids	Reported in tonnes	N/A	N/A	12668	N/R	N/R	N/R
Herbicides	36741000	Product Grouping too variable			N/R	N/R	N/R
Paints, varnish, laquers	142863000	1[a]	142863000	142,863	158,000*	55,000*	102,000*
Household products – candles, oils	29,796,000	Grouping too variable			N/R	N/R	N/R

TABLE 2-2: Production volumes for organic related chemicals in South Africa (*contd.*)

STATS SA P3051.3 Feb 2003					STATS SA P3051.3 Feb 2002 (DEAT (a), 2003)	SARS Customs & Excise (DEAT (a), 2003)	
						Import	**Export**
Product	**Liters**	**SG**	**Kilograms**	**Tonnes**	**Tonnes**	**Tonnes**	**Tonnes**
Soaps, detergents, polishes, wax	Reported in tonnes	(N/A)	N/A	468,085	565,000	45,000	81,000
Soaps, detergents, polish (liquid)	131,245,000	0.906 – 0.942[b] (Waxes) 0.924 – 0.96[c] (oils)	27,799,668	27,799.668	N/R	N/R	N/R
Cosmetics, toiletries	Reported in tonnes	N/A	N/A	16,618	N/R	N/R	N/R
Cosmetics, toiletries (liquid)	26,194,000	Grouping too variable			N/R	N/R	N/R
Pharmaceuticals (ointments)	Reported in tonnes	N/A	N/A	5259.2	N/R	N/R	N/R
Pharmaceuticals (ointments)	1,276,000	Grouping too variable			N/R	N/R	N/R
Petroleum Products							
Motor Spirit (Octane, petrol)	10,396,000,000	0.7-0.76[d]	7,589,080,000	7,589,080	N/R	N/R	N/R
Aviation Spirit	3,104,184,000	0.62-0.88[c]	2,328,138,000	2,328,138	N/R	N/R	N/R
Fuel oil (Diesel)	7,654,000,000	0.82-0.86[d]	6,429,360,000	6,429,360	N/R	N/R	N/R
Lubricating and process oils	Reported in tonnes	N/A	N/A	10,571	N/R	N/R	N/R

TABLE 2-2: Production volumes for organic related chemicals in South Africa (*contd.*)							
STATS SA P3051.3 Feb 2003					**SARS Customs & Excise (DEAT (a), 2003)**	**SARS Customs & Excise (DEAT (a), 2003)**	
						Import	**Export**
Product	**Liters**	**SG**	**Kilograms**	**Tonnes**	**Tonnes**	**Tonnes**	**Tonnes**
Liquid petroleum gas	Reported in tonnes	N/A	N/A	498,090	N/R	N/R	N/R
Total	Reported in tonnes	N/A	N/A	*17,464,226*	17,115,000**	19,491,000**	62,338,000**
Polymers and plastics							
Plastic – primary forms	Reported in tonnes	N/A	N/A	829,384	N/R	N/R	N/R
Tyres	Reported in tonnes	N/A	N/A	21,378	N/R	N/R	N/R
Pipes	Reported in tonnes	N/A	N/A	1,714	N/R	N/R	N/R
Bags	Reported in tonnes	N/A	N/A	112,772	N/R	N/R	N/R
Containers	Reported in tonnes	N/A	N/A	73,918	N/R	N/R	N/R
Hoses, pipes	Reported in tonnes	N/A	N/A	42,363	N/R	N/R	N/R
Packaging	Reported in tonnes	N/A	N/A	28,579	N/R	N/R	N/R
Total	Reported in tonnes	N/A	N/A	*1,110,108*	793,000***	427,000	458,000
Glues, starches	Reported in tonnes	N/A	N/A		201,000	40,000	6,000
Explosives	Reported in tonnes	N/A	N/A			4,000	33,000

A General Paint (2003)
B Zophar Mills (2003)
C CSG Network (2003)
D Sasol Index (2003)

* *Liters of paints, varnishes & lacquers converted to tonnages by using an SG of 1.*
** *Petroleum products converted to tonnages by using an average SG of 0.8005.*
*** *Total of polymers and plastics may have been under-estimated by DEAT (Feb 2002 stats) – included in the STATSSA 2003 figure together with plastic products is raw plastics.*

From the above the following can be deduced:

- A combined figure of approximately 90 *million tonnes* of petroleum and organic related chemicals and products are produced and imported annually into South Africa. According to CAIA (2002) a figure of 13 *M tonnes* of chemicals (organic and inorganic) are produced annually in South Africa. This figure seems to include petroleum (fuel) and related products.
- Petroleum products show the highest production figure (95%) – see **FIGURE 2-1**.
- The rest of the products are roughly in the same range (from 0.01% up to 2%)
- The following products may have been under-estimated due to volumes that were given in litres that could not be satisfactorily converted to tonnages. The reason for this is that the SG's of the product grouping (insecticides and herbicides) or the grouping itself (cosmetics and toiletries) were too variable:
    - Insecticides and herbicides
    - Liquid cosmetics and toiletries
    - Pharmaceutical ointments

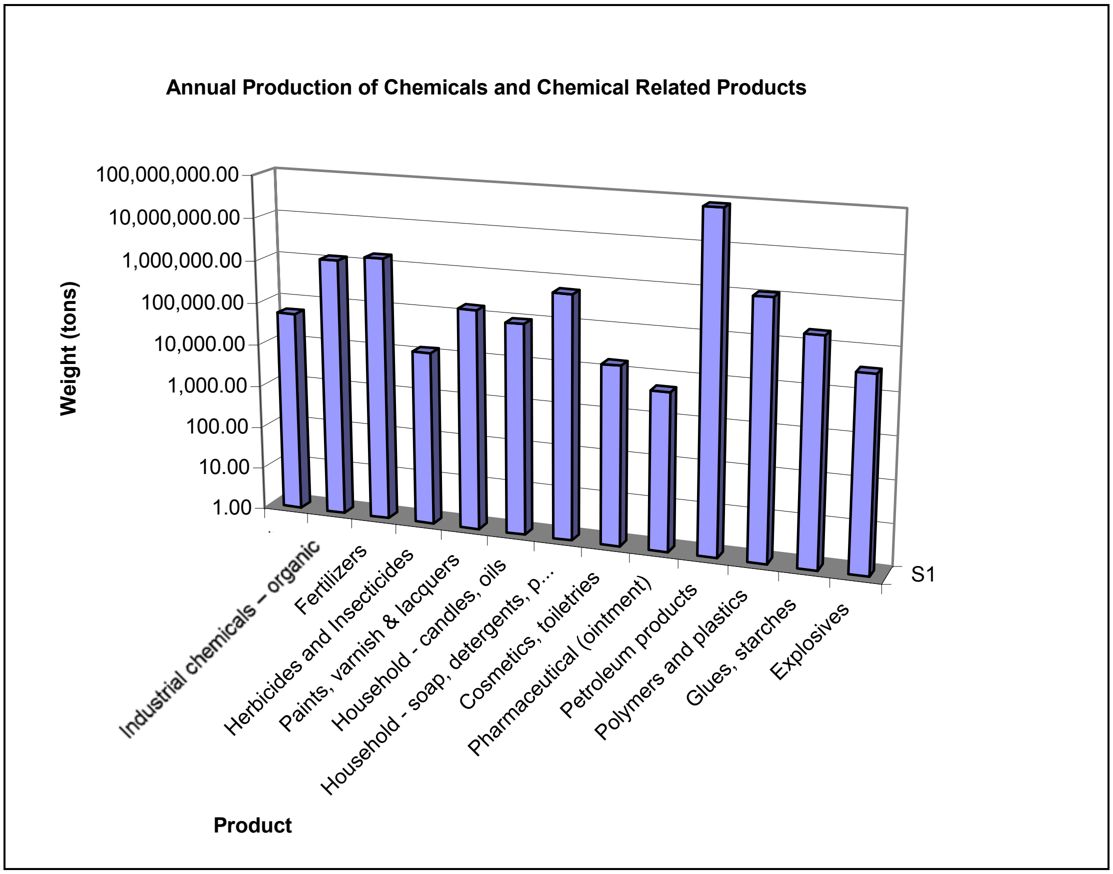


Figure 2-1 (Annual production of chemicals and chemical related products)

To check whether the petroleum product information is correct, the following statistics have also been gathered:

The petroleum industry:

South Africa contributes 791 thousand metric tonnes of crude oil to the South African Petroleum Industries Association (SAPIA), where the total contribution of crude oil to SAPIA from all the associated members, is 18,896 thousand metric tonnes (SAPIA (a), 2002). Petroleum products production volumes can be measured against annual sales, which, for South Africa, can be seen in **TABLE 2-3** (SAPIA (b), 2002):

TABLE 2-3: Product Volumes of Sales in millions of Litres

	Jan to Dec 2000	**Jan to Dec 2001**	**Jan to Dec 2002**
Petrol	10396	10340	10335
Diesel	6254	6488	6831
Jet Fuel	2020	1924	1967
Illuminating Paraffin	857	786	745
Fuel Oil	555	555	536
Bitumen	219	242	267
LPG	567	599	586
Total	*20868*	*20934*	*21267*

This means that approximately 21 billion litres, or using a SG of 0.8005*, that 17 million tonnes of petroleum related products are sold annually in SA. This relates well to the figure of between 17 and 19 million tonnes of petroleum products production in South Africa (**TABLE 2-2**). The extra 62 million tonnes is exported, making up a total of almost 80 million tonnes of petroleum and related products that must reside in the country annually. Although the production of petroleum products (petrol, diesel etc.) makes up 95 per cent of production figures for organic related products, the pollution sources of this product will be limited to filling stations selling the product, pipelines that transport this fuel, and industries and mines that use and store the product in large quantities. An estimate of filling stations existing in South Africa currently; is given in section 2.1.6.1 (land-use activities associated with organic pollution) in an effort to quantify an amount of point sources for possible pollution from filling stations. The other 5 per cent represented by industries, is more readily quantifiable and is as relevant as filling station pollution, in that the industries introduce complex NAPLs into aquifer systems (due to processing occurring at industries), as opposed to filling stations that introduce on the most part LNAPL pollution, which can be more easily remediated than DNAPL and other complex NAPLs. Certain urban activities also contribute to organic pollution and are highlighted in section 2.1.6.1.

* The SG of 0.8005 was derived by adding and averaging the SGs for Motor Spirit (Octane, petrol) - 0.7-0.76 (Sasol Index, 2003), Aviation Spirit - 0.62-0.88 (CSG Network, 2003), Fuel oil (Diesel) - 0.82-0.86 (Sasol Index, 2003) and Lubricating and process oils (grease) - 0.86-0.904 (CSG Network, 2003).

2.1.6 Pollution sources

2.1.6.1 Land use activities that are associated with organic pollution

TABLE 2-4 list organic pollutants typically associated with certain urban activities, which can be analyzed for if pollution is suspected. The information has been obtained from MDEP (1999) and WRC (2004).

TABLE 2-4: Organic pollutants associated with urban activities

Organic chemical	Airports	Auto repair shops	Car washes	Cemeteries	Dry cleaners	Furniture stripping	Medical facilities	Paint shops	Photo processors	Gas / Service stations
acenapthene		✓								✓
acenapthylene		✓								✓
acetone	✓	✓				✓	✓	✓		✓
anthracene		✓								✓
benzene	✓	✓	✓			✓	✓	✓		✓
Benzo(a)anthracene		✓								✓
Benzo(a)pyrene		✓								✓
Benzo(b,j,k)fluoranthene		✓								✓
Benzo(g,h,i)perylene		✓								✓
bromobenzene	✓	✓								
bromoform							✓			
carbon tetrachloride	✓					✓		✓		
chloride		✓						✓		
chlorobenzene	✓	✓				✓		✓		✓
chloroethene		✓								
chloroform							✓			
chrysene		✓								✓
cumene	✓									
dichlorofluoromethane								✓		
dichlorodifluoromethane		✓					✓			✓
diethylphtalate									✓	
Di(2-ethylhexyl)phtalate								✓		
dimethylpthalate						✓		✓		
ethylbenzene	✓	✓	✓			✓		✓		✓
fluoranthene		✓								✓
fluorine		✓								✓
fluorotrichlorometane										✓
hexachlorobutadiene	✓	✓								
hexylphtalate								✓		
methylene		✓						✓		
Methylene chloride						✓				✓

TABLE 2-4: Organic pollutants associated with urban activities *(contd..)*										
Organic chemical	**Airports**	**Auto repair shops**	**Car washes**	**Cemeteries**	**Dry cleaners**	**Furniture stripping**	**Medical facilities**	**Paint shops**	**Photo processors**	**Gas / Service stations**
MTBE			✓				✓			
n-propylbenzene	✓	✓								
naphthalene	✓	✓	✓							✓
nitrobenzene							✓			
o-dichlorobenzene		✓				✓		✓		✓
p-dichlorobenzene							✓			
pentachlorophenol				✓		✓	✓			
phenanthrene	✓	✓					✓			✓
phenol		✓		✓		✓	✓	✓	✓	
PCB		✓								✓
PCE	✓				✓			✓		
pyrene		✓								✓
styrene							✓			
TCE	✓	✓			✓	✓	✓	✓		✓
tetrachloroethylene		✓								✓
trichlorometane								✓		
trichlorofluoromethane							✓			
toluene	✓	✓	✓			✓	✓	✓		✓
VOC	✓	✓	✓		✓	✓		✓	✓	✓
xylene	✓	✓	✓			✓		✓		✓
1,1 DCA	✓	✓				✓	✓	✓		✓
1,1 DCE						✓	✓			
1,1,1 TCA	✓	✓			✓	✓		✓		✓
1,1,1,2-tetrachloromethane							✓			
1,1,2,2 tetrachloroethane	✓					✓		✓		
1,2 DCA	✓	✓				✓		✓		✓
1,2 DCE	✓					✓		✓		
1,2-dichloropropane		✓			✓	✓		✓		✓
1,4-diphenylhydrazine							✓			
1,2,3 trichlorobenzene		✓								✓
1,2,4 trimethylbenzene	✓	✓	✓					✓		✓
1,3-dichloropropane							✓			
1,3,5 trimethylbenzene	✓									
2-methylnaphthalene	✓	✓	✓							✓
2-methylphenol							✓			✓
2,4-Dichlorobenzene	✓									
2,4-dinitrophenol							✓		✓	
2,4,6-trichlorophenol							✓			

In **TABLE 2-5**, below, the industries that were plotted on the map of South Africa (see Section 2.1.7, specifically Section 2.1.7.3) are given together with possible organic pollutants associated with these industries. Again, these chemicals serve as fingerprinting chemicals for certain industries.

TABLE 2-5: Organic pollutants associated with industries

Organic chemical	**Metal casting**	**Structural metals manufacturing**	**Fabricated metal Metal services**	**Food preservation**	**Beverages production**	**Textiles**	**Dressing & dyeing of fur**	**Coal & lignite mining**	**Crude petrol extraction**	**Iron ore mining**	**Tanning & dressing Of leather**	**Paper manufacturing**	**Petroleum refineries & synthesizers**	**Basic chemicals manufactuing**	**Other chemicals produciton**	**Rubber products manufacturing**	**Plastic manufacturing**	**Basic Iron & steel manufacturing**
acenapthene									✓				✓					
acenapthylene									✓				✓					
acetone	✓	✓	✓											✓	✓	✓	✓	✓
anthracene									✓		✓		✓					
benzene							✓	✓		✓	✓			✓	✓			✓
Benzo(a)anthracene									✓				✓					
Benzo(a)pyrene									✓				✓					
Benzo(g,h,i)perylene									✓				✓					
bromobenzene														✓	✓			
butadiene																✓	✓	
butane																		
carbon tetrachloride	✓	✓	✓											✓	✓			
chlorobenzene	✓	✓	✓											✓	✓			✓
chloroform														✓	✓			
chrysene									✓				✓					
cumene														✓	✓			
dichlorobenzene														✓	✓			
dichlorofluoromethane																✓	✓	

TABLE 2-5: Organic pollutants associated with industries *(contd.)*

Organic chemical	Metal casting	Structural metals manufacturing	Fabricated metal Metal services	Food preservation	Beverages production	Textiles	Dressing & dyeing of fur	Coal & lignite mining	Crude petrol extraction	Iron ore mining	Tanning & dressing Of leather	Paper manufacturing	Petroleum refineries & synthesizers	Basic chemicals manufactuing	Other chemicals produciton	Rubber products manufacturing	Plastic manufacturing	Basic Iron & steel manufacturing
dichlorodifluoromethan	✓	✓																
diethylphtalate														✓	✓			
Di(2-ethylhexyl)phtalat	✓	✓									✓			✓	✓			
dimethylpthalate	✓	✓									✓							
Ethyl acetate						✓												
ethylbenzene	✓	✓	✓					✓		✓				✓	✓	✓	✓	
ethanol					✓													
fluorine									✓				✓					
formaldehyde																✓	✓	
hexachlorobutadiene														✓	✓			
methane				✓	✓									✓	✓			
Methylene chloride	✓	✓	✓											✓	✓			
MTBE														✓	✓			
naphthalene	✓	✓	✓					✓	✓	✓	✓		✓	✓	✓			
nitrobenzene			✓											✓	✓			
o-dichlorobenzene	✓	✓	✓								✓			✓	✓			
p-dichlorobenzene											✓			✓	✓			
pentachlorophenol											✓							
phenanthrene								✓	✓	✓	✓		✓					
phenol	✓	✓	✓	✓	✓	✓	✓		✓			✓	✓	✓	✓	✓	✓	✓
PCE	✓	✓	✓											✓	✓	✓	✓	
pyrene									✓				✓					

TABLE 2-5: Organic pollutants associated with industries *(contd.)*

Organic chemical	Metal casting	Structural metals manufacturing	Fabricated metal Metal services	Food preservation	Beverages production	Textiles	Dressing & dyeing of fur	Coal & lignite mining	Crude petrol extraction	Iron ore mining	Tanning & dressing Of leather	Paper manufacturing	Petroleum refineries & synthesizers	Basic chemicals manufactuing	Other chemicals produciton	Rubber products manufacturing	Plastic manufacturing	Basic Iron & steel manufacturing
styrene	✓	✓	✓											✓	✓	✓	✓	
TCE	✓	✓	✓											✓	✓	✓	✓	
tetrachlorobenzene														✓	✓			
tetrachloroethylene																		✓
trichlorobenzene														✓	✓			
trichlorofluoromethane	✓	✓	✓															
toluene	✓	✓	✓			✓	✓	✓		✓	✓	✓		✓	✓	✓	✓	
Vinyl chloride																✓	✓	
xylene	✓	✓	✓	✓	✓	✓	✓	✓		✓		✓		✓	✓			
1,1 DCA	✓	✓	✓											✓	✓			
1,1,1 TCA	✓	✓	✓											✓	✓			✓
1,1,2,2 tetrachloroethan			✓											✓	✓			
1,2 DCA	✓	✓	✓											✓	✓			
1,2 DCE														✓	✓			
1,2-dichloropropane	✓	✓	✓											✓	✓			
1,2,3 trichlorobenzene														✓	✓			
1,2,4 trimethylbenzene																✓	✓	
1,3-dichloropropane														✓	✓			
2-methylnaphthalene								✓	✓	✓			✓	✓	✓			
2-methylphenol									✓				✓					
2,4,6-trichlorophenol											✓			✓	✓			
Total Assoc. Chemicals	21	21	22	3	4	4	4	7	14	7	11	3	14	37	37	12	12	6

A risk factor was coupled to the industries in **TABLE 2-5** in order to derive an indication of risk associated with each industry. The risk factor has been determined from the amount of associated organic contaminants. The other activities also pose risk, but less so because of a lower amount of associated organic chemicals. This information will be used in Section 2.2.3 during the determination of the aquifer vulnerability. This risk is by no means the total associated risk. The fact that interacting toxic effects could not be included in this risk factor (since it is still to a large degree an unknown to chemical medical science profession), is a limitation. From **TABLE 2-5** it could be concluded that the industrial activities posing the greatest risk (given in descending order) are: Basic chemical manufacturing, other chemical manufacturing, fabricated metal & metal services, structural metals manufacturing, metal casting, petrol refining, crude petrol extraction, plastic manufacturing, rubber manufacturing, tanning and dressing of leather, coal and lignite mining and iron ore mining. The following statistics could shed light on the problem South Africa is facing in terms of organic point source pollution via service stations. The market share (in 2001) for the different companies was divided as can be seen in **TABLE 2-6** (SAPIA (c), 2002):

TABLE 2-6: 2001 Market shares for different oil companies

Company	**Diesel**	**Oil**
Afric Oil	0,04	0,99
BP	16,24	15,73
Caltex	17,43	16,69
Engen	27,02	27,25
Exel	2,23	4,84
Sasol	6,06	0,85
Shell	17,53	17,80
Tepco	0,33	2,22
Total	13,12	13,63
Percentage	100	100

Figures on service stations in South Africa have been obtained, and are shown in **TABLE 2-7**.

TABLE 2-7: Number of service stations per South African fuel provider

Company	**Amount of Service Stations *(real figures)***	**Estimated Amount of Service Stations *(rounded to the nearest 100)***
Engen	1914 [a]	1900
BP	800 [b]	800
Total	564 [c]	600
Caltex		800
Shell		800
Exel & Sasol		300
Totals (*rounded to the nearest 100*)	3300	5200

a Engen (2003), b BP (2003), c Total (2003)

Taking firstly into account only Engen and BP's real figures and the market shares of the different companies, it was estimated what amount of service stations Total and the other companies should have. A rounded figure of 600 was obtained for Total. After obtaining information on the amount of service stations that Total has (from an updated website) it could be confirmed that estimating the amount of service stations from the market shares is reasonably correct.

From **TABLE 2-7** it can be deduced that there exist at least 3300 known service stations with the possibility of 5200 service stations that may represent point organic pollution sources. The pollution occurs because most of the underground storage tanks have corroded away over the years and now leak petrol and diesel. These point pollution sources will be spread over the whole country – where towns are situated and all along the major highways. Towns overlying aquifer vulnerable areas, and which rely on ground water for its sole water resource, will have to be identified and the service station of those towns have to be checked for tank leakages, and if identified, have to be serviced with new underground storage tanks.

2.1.6.2 Industrial waste generation in South Africa

It has been seen in section 2.1.6.1 that several sources of organic pollution exist, and that identification and quantification of these sources is of cardinal importance for aquifer management and protection. In order to show the level of knowledge the authorities currently possess on industrial pollution in general; and what contribution industrial waste makes towards annual waste production in South Africa, **TABLE 2-8** is given below. **TABLE 2-8** list volumes of waste produced per waste stream (DEAT (a), 2003).

TABLE 2-8: Volumes of waste produced per waste stream in South Africa

Waste stream	**Generation Million t/a**
Mining	468.2
Industrial	16.3
Power Generation	20.6
Agriculture and Forestry	20
Domestic and Trade	8.2
Sewage sludge	0.3
Total	*533.6*

From **TABLE 2-8** it can be seen that mining contributes the most waste, followed by industries. DWAF (a), 1998, highlights a lack of information regarding industrial waste that is disposed of on site (DEAT (a), 2003). Industries account for most hazardous waste, and of the 5 million cubic meters of hazardous waste generated every year, less than 5% reaches hazardous waste disposal sites (UNEP, 2003). Furthermore, the rate of increase in production of hazardous waste is estimated to be 2.6% per annum over the next 10 years (UNEP, 2003). There are currently seven operational commercial hazardous disposal sites in South Africa. (Le Roux, 2003). However, there are several industries with their own sites which accept just waste from their plants. There are approximately 30 such sites permitted in South

Africa. In total one million tonnes of industrial hazardous waste is being disposed of the abovementioned sites (Le Roux: *personal communication*, 2003). As can be seen, a large gap in knowledge exists regarding industrial waste generation in general, and regarding organic waste generation in particular, with huge amounts of waste (some constituting organic waste) being unaccounted for. The hazardous waste does, however, not only end up at these waste sites, but is sometimes dumped at lower class waste sites (e.g. domestic waste sites). Transport of this waste also poses problems. Some trucks are not adequately equipped to carry of waste and a large amount of accidents occur regularly where the hazardous chemical waste is spilled. Cleanup of these spills is the responsibility of the fire departments and only major towns and cities have fire departments. This leaves large stretches of the N1 highway without fire departments and a resultant problem with cleanup if a spill occurs.

2.1.7 Positions of the different industries in South Africa, shown in terms of intensity of industrial activity

2.1.7.1 Information source

The information used to compile the industrial maps, has been obtained from Statistics South Africa's Cencus 2001 survey (STATS SA (a), 2001). Six levels of information were captured and stored on the Cencus Spatial Database, which the Sub Place Names (Level 6) were used. Standard Industrial Code (SIC) information for the whole of South Africa was obtained from STATS SA, and these two entities were linked to generate the industrial maps. Only these two entities will be explained (definitions given below) in detail since they were used in the compilation of the industrial maps.

Sub Places Names

This is level 6 in the place name hierarchy. In some cases a sub place and type is not defined; where 'NONE' is used to denote such occurrences. An eight-digit geo-code was generated for each sub place (STATS SA (b), 2001): **The first digit** *denotes the province;* **the second and third digits** *denote the municipality;* **the fourth and fifth digits** *identify the main place, while* **the last three digits** *identify a unique sub place within the main place.* The last five digits therefore identify a unique sub place within a municipality.

The Standard industrial classification (SIC) - (STATS SA, 1993):

The SIC was designed for the classification of establishments according to the kind of economic activity, and provides a standardized framework for the collection, tabulation, analysis and presentation of statistical data on establishments. An industry consists of establishments engaged in the same or a closely related kind of economic activity based mainly on the principal class of goods produced or services rendered. The SIC coding system use numbers to identify the major divisions, divisions, major groups, groups and subgroups are arranged according to a decimal system.

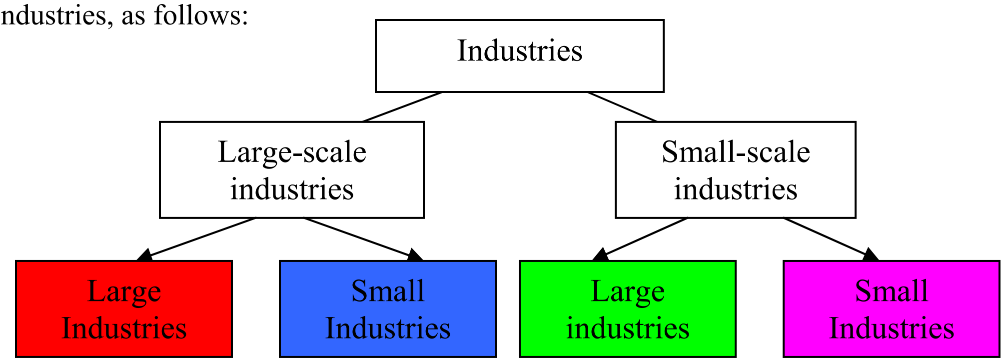
2.1.7.2 Method for the compilation of the industrial maps

In order to compile industrial maps (**FIGURES 2.2 – 2.20**), the sub place name information was linked with the major group SIC's listed in **TABLE 2-9**.

TABLE 2-9: Major groups of industrial activities used for compilation of industrial maps

Code	**Explanation**
210	Mining Of Coal And Lignite
221	Extraction Of Crude Petroleum & Natural Gas; Oil & Gas Exploration Service Activities
241	Mining Of Iron Ore
301	Production; Processing And Preservation Of Meat; Fish; Fruit; Vegetables; Oils And Fats
305	Manufacture Of Beverages
311	Spinning; Weaving And Finishing Of Textiles
315	Dressing And Dyeing Of Fur; Manufacture Of Articles Of Fur
316	Tanning & Dressing Of Leather; Manufacture Of Luggage; Handbags; Saddlery & Harnesses
323	Manufacture Of Paper And Paper Products
332	Petroleum Refineries/Synthesizers
334	Manufacture Of Basic Chemicals
335	Manufacture Of Other Chemical Products
337	Manufacture Of Rubber Products
338	Manufacture Of Plastic Products
351	Manufacture Of Basic Iron And Steel
353	Casting Of Metals
354	Manufacture Of Structural Metal Products; Tanks; Reservoirs And Steam Generators
355	Manufacture Of Other Fabricated Metal Pro-Ducts; Metalwork Service Activities

The data for each of the above listed industrial codes that is associated with each sub place name code have been extracted for the whole South Africa. The 2001 spatial data sub place codes all have associated polygons, sub place names and coordinates (latitude, longitude). The SP_codes of the Standard Industrial Classification (SIC's) have been linked with the SP_codes on the Census 2001 spatial database. The linked files were then plotted over the South African provincial boundary data (from Metalmap, 2001) in order to obtain the final industrial maps. The industries were divided into two categories – large-scale industries and smaller scale industries. These two categories were again divided into two classes – large and small industries, as follows:



The colour signifies the size of the industry, and the same colours have been used in creating the industrial maps, as can be seen in the legend to the maps in the section covering the results.

Large-scale industries:

Large-scale industries for the purpose of this exercise; employ larger amounts of people than the smaller scale industries. The scale of the industry is not necessarily associated with the annual production and export volumes of these industries, but may coincide. Typical employment figures, obtained from STATS SA, for the following industries, are from a few hundred to a few thousand people per industry.

List of large-scale industries:

Coal and lignite mining, Iron Ore Mining, Food Preservation, Manufacture of Beverages, Preparation, spinning and weaving of textiles, Tanning and Dressing of leather, Manufacture of Paper and Paper Products, Petroleum Refineries and Synthesizers, Manufacture of basic chemicals, Production of other chemicals, Manufacture of rubber products, Manufacture of plastic, Basic Iron and Steel Manufacturing, Casting of Metals, Manufacturing of Steel Products, Fabricated Metal and Metal Services.

Small-scale industries:

The smaller scale industries typically employ up to a few hundred people per industry.

List of small-scale industries:

Crude Petrol Extraction, Dressing and Dyeing of fur

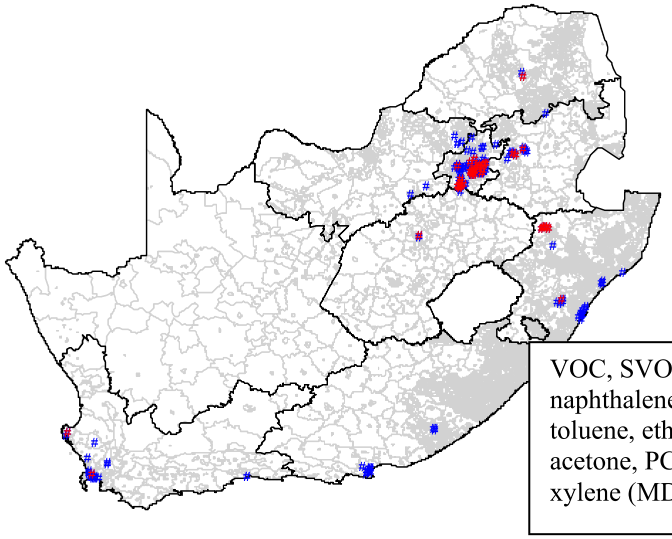
2.1.7.3 Results

The generated industrial maps are shown below in **FIGURES 2-2** to **2-20**. In a text box below each map, the organic variables most likely to be found as contaminants are listed. These do not represent all the contaminants that can be found in association with the specific industry.

Legend to maps

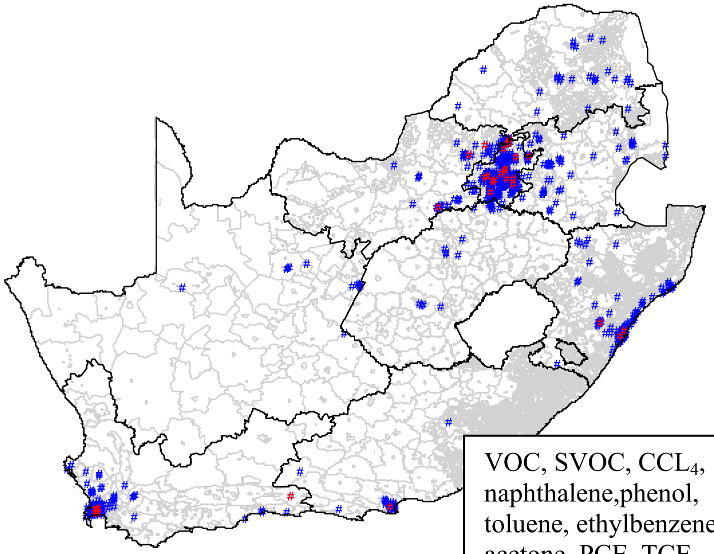
🟥	> 25 persons active / selected industry
🟦	> 5 persons active / selected industry
🟩	> 15 persons active / selected industry
🟪	> 1 persons active / selected industry
🟩	Coal mining area (Metalmap, 2001)
🟧	Active & dormant collieries (Metalmap, 2001)
▨	Provincial boundaries

Figure 2-2 353 Casting of metals:



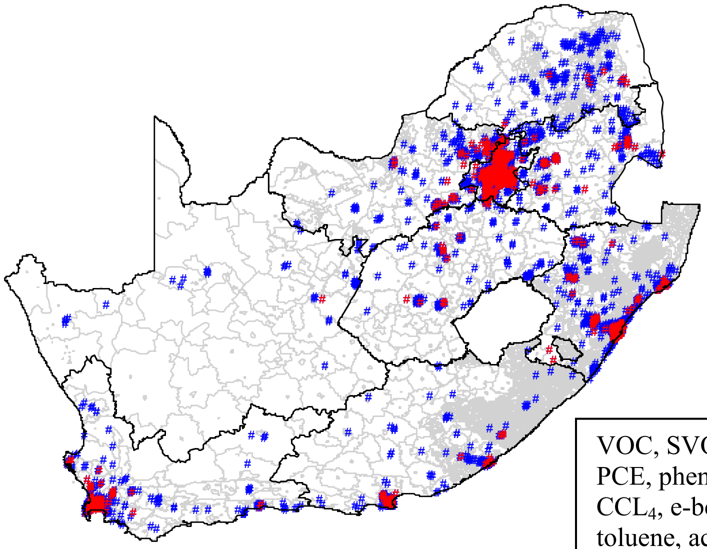
VOC, SVOC, CCL$_4$, naphthalene,phenol, toluene, ethylbenzene, acetone, PCE, TCE, xylene (MDEP, 1999)

Figure 2-3 354 Manufacture of structural metal products:



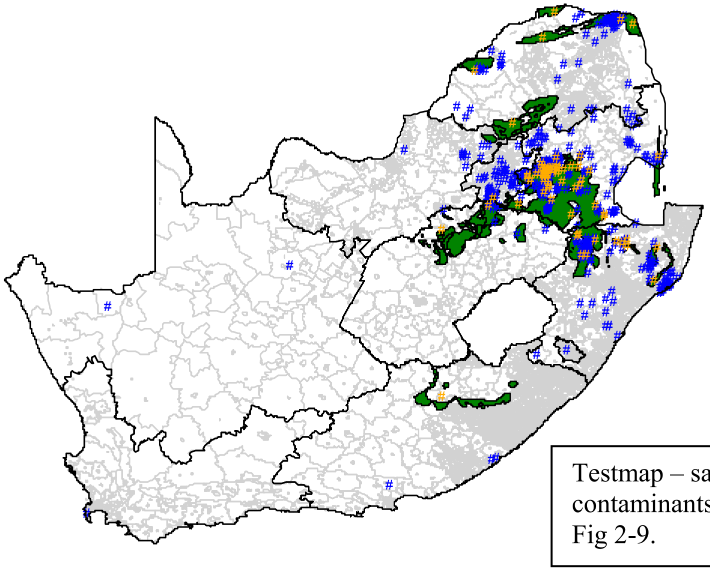
VOC, SVOC, CCL$_4$, naphthalene,phenol, toluene, ethylbenzene, acetone, PCE, TCE, xylene (MDEP, 1999)

Figure 2-4 355 Fabricated Metal, Metal Services:



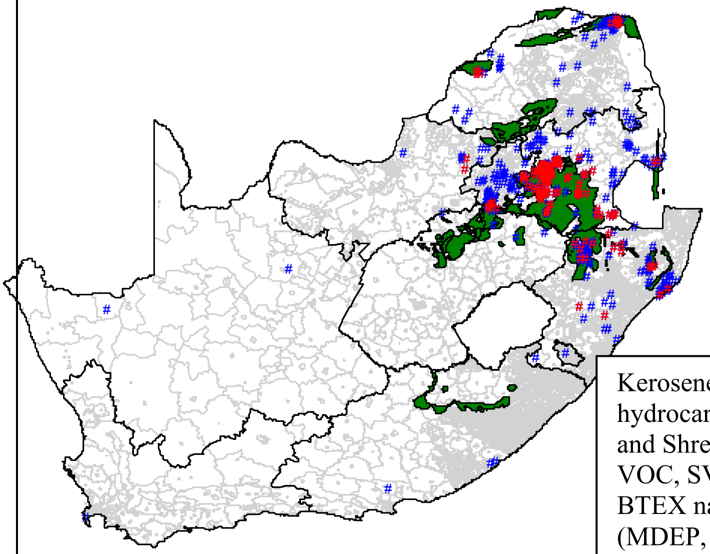
VOC, SVOC, PCE, phenol, CCL$_4$, e-benzene, toluene, acetone, (MDEP, 1999)

Figure 2-5 Coal Metalmap:



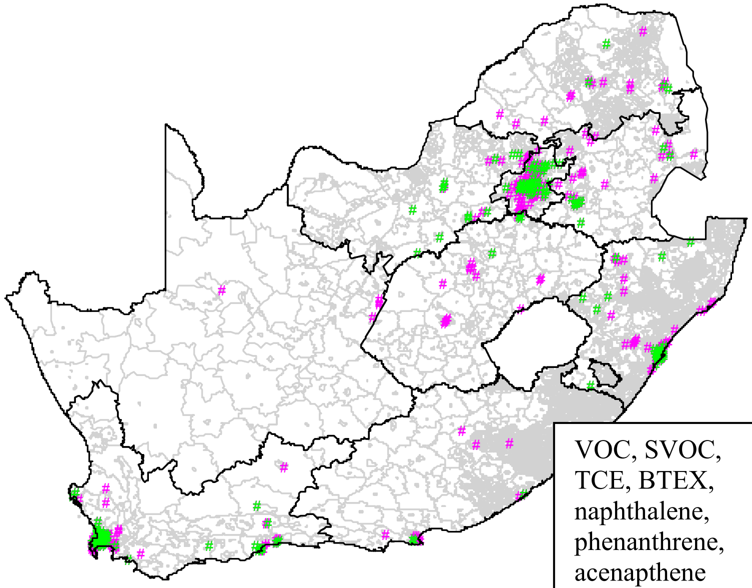
Testmap – same contaminants as Fig 2-9.

Figure 2-6 210 Coal and lignite mining:



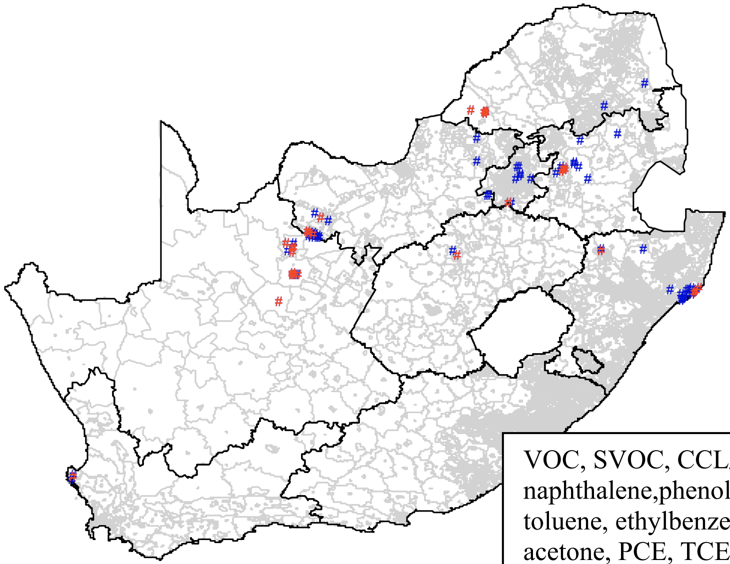
Kerosene, hydrocarbons (Brink and Shreve, 1977) VOC, SVOC, BTEX naphthalene (MDEP, 1999)

Figure 2-7 221 Crude petrol extraction:



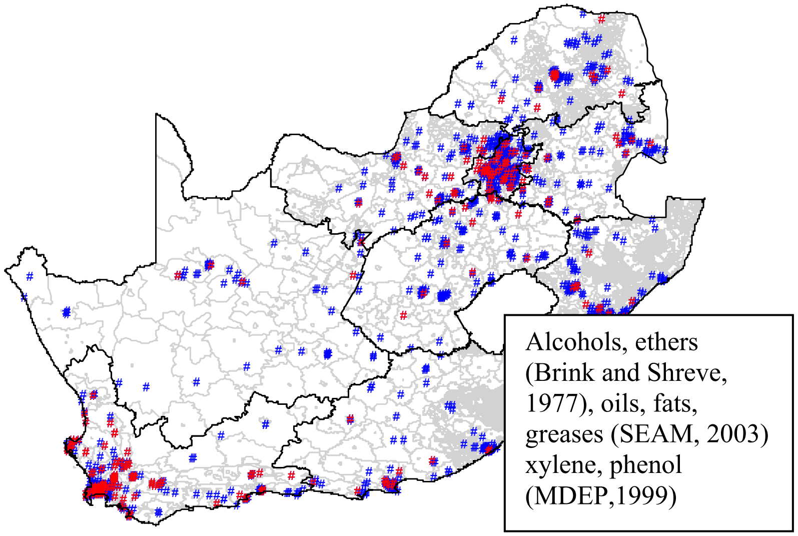
VOC, SVOC, TCE, BTEX, naphthalene, phenanthrene, acenapthene (MDEP, 1999)

Figure 2-8 241 Iron ore mining:



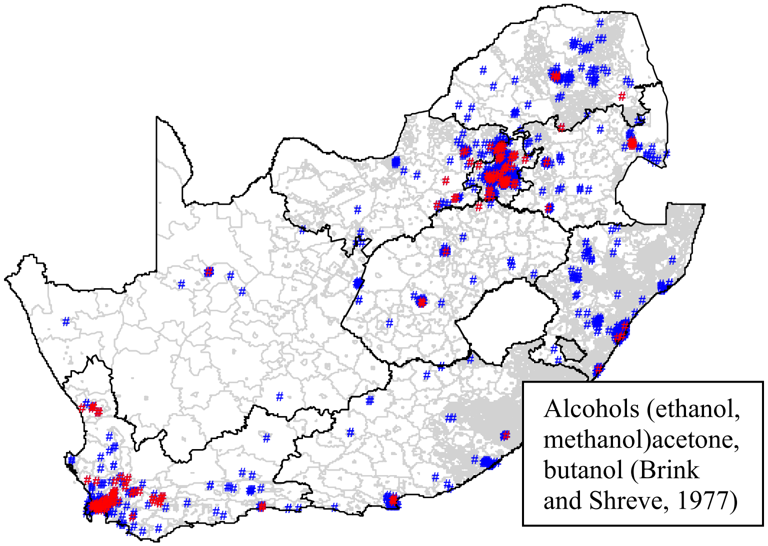
VOC, SVOC, CCL_4, naphthalene,phenol, toluene, ethylbenzene, acetone, PCE, TCE, xylene (MDEP, 1999)

Figure 2-9 301 Food preservation:



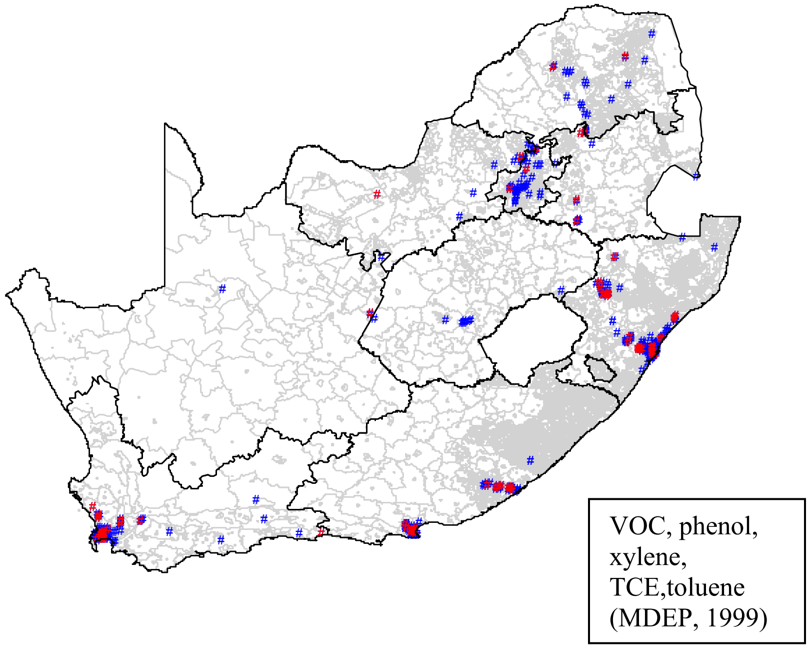
Alcohols, ethers (Brink and Shreve, 1977), oils, fats, greases (SEAM, 2003) xylene, phenol (MDEP,1999)

Figure 2-10 305 Manufacture of beverages:



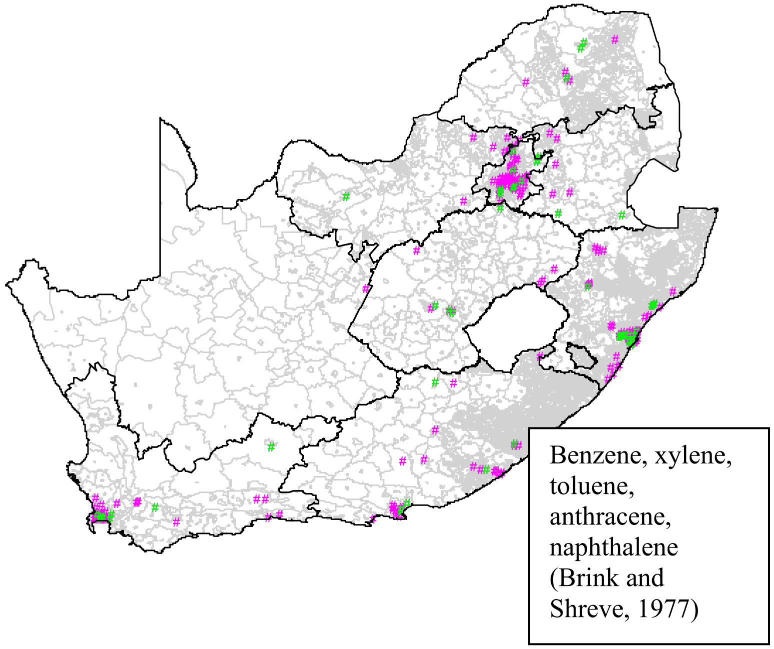
Alcohols (ethanol, methanol)acetone, butanol (Brink and Shreve, 1977)

Figure 2-11 311 Preparation, Spinning & Weaving of Textiles:



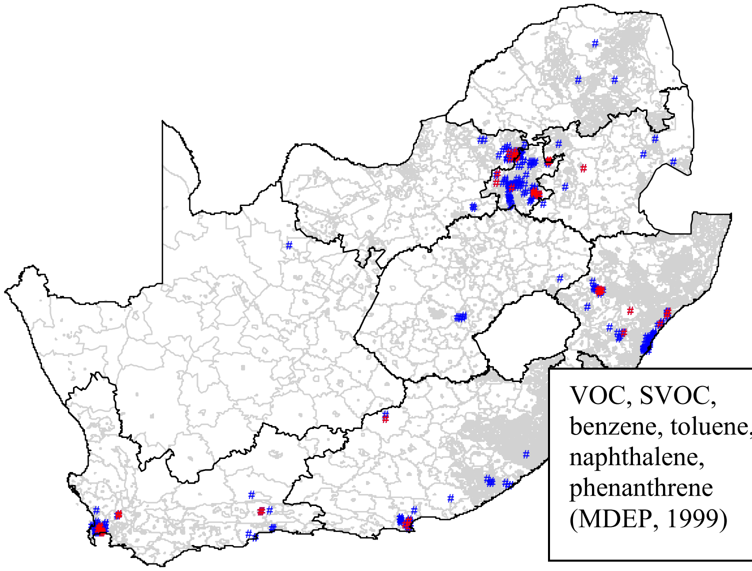
VOC, phenol, xylene, TCE,toluene (MDEP, 1999)

Figure 2-12 315 Dressing & Dyeing of fur:



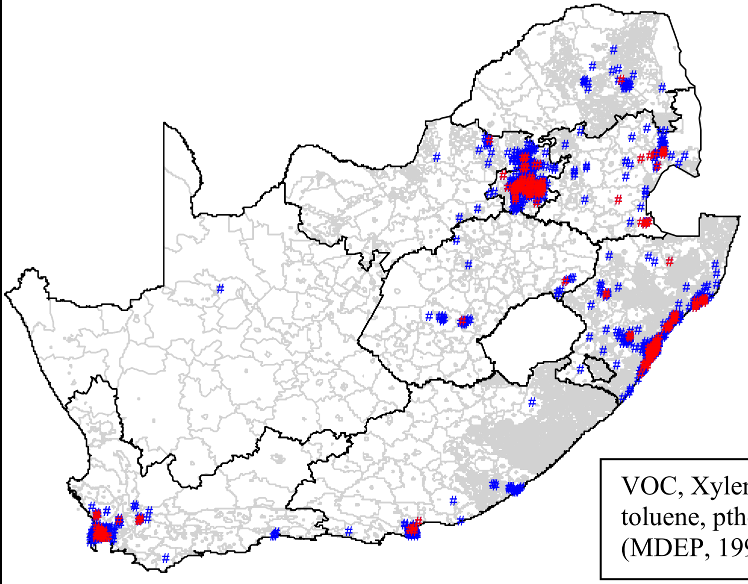
Benzene, xylene, toluene, anthracene, naphthalene (Brink and Shreve, 1977)

Figure 2-13 316 Tanning & Dressing of leather:



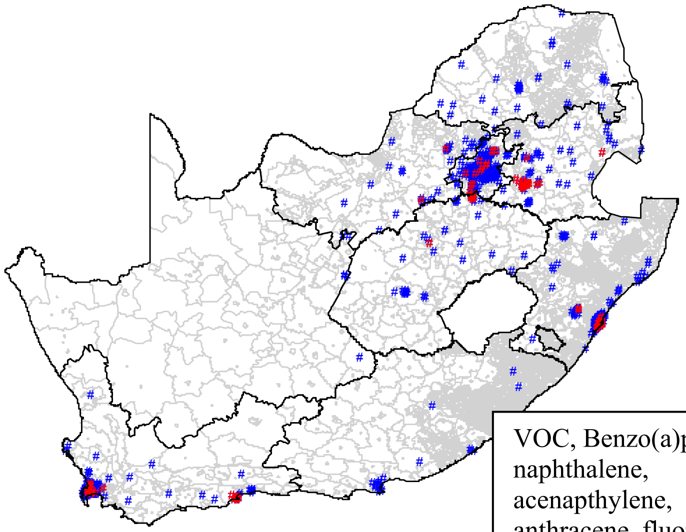
VOC, SVOC, benzene, toluene, naphthalene, phenanthrene (MDEP, 1999)

Figure 2-14 323 Manufacture of Paper & Paper products



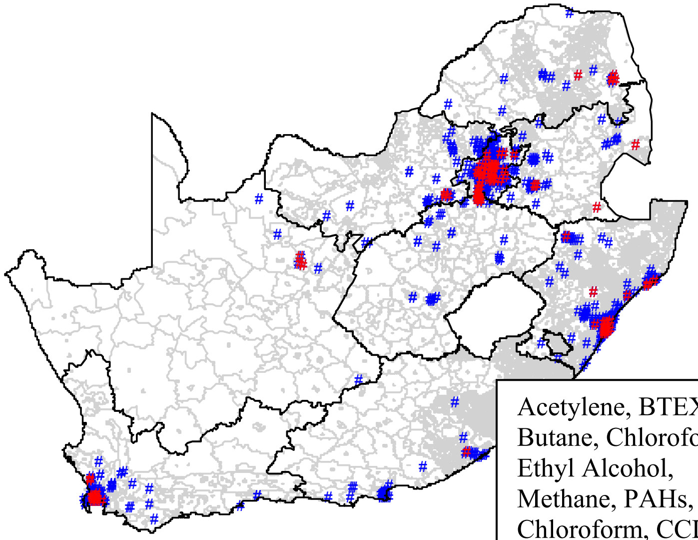
VOC, Xylene, toluene, pthenol (MDEP, 1999)

Figure 2-15 332 Petroleum Refineries and Synthesizers:



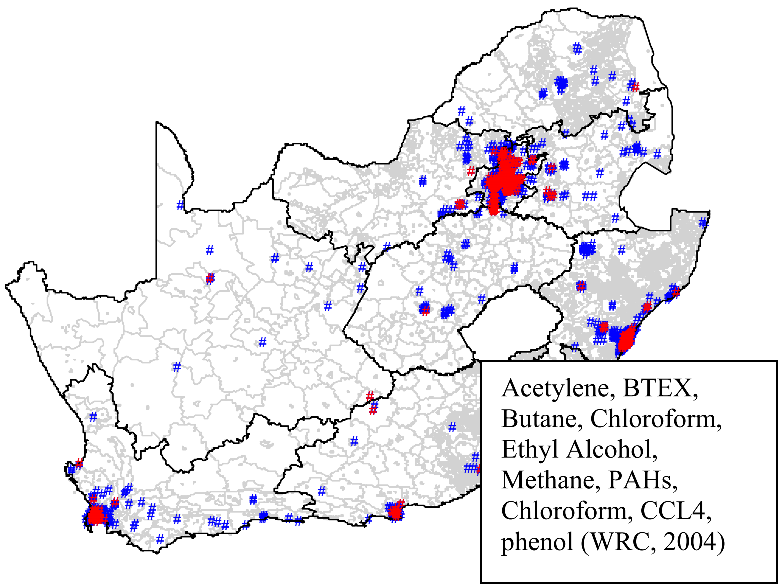
VOC, Benzo(a)pyrene, naphthalene, acenapthylene, anthracene, fluorine, phenanthrene, phenol (MDEP, 1999)

Figure 2-16 334 Manufacture basic chemicals:



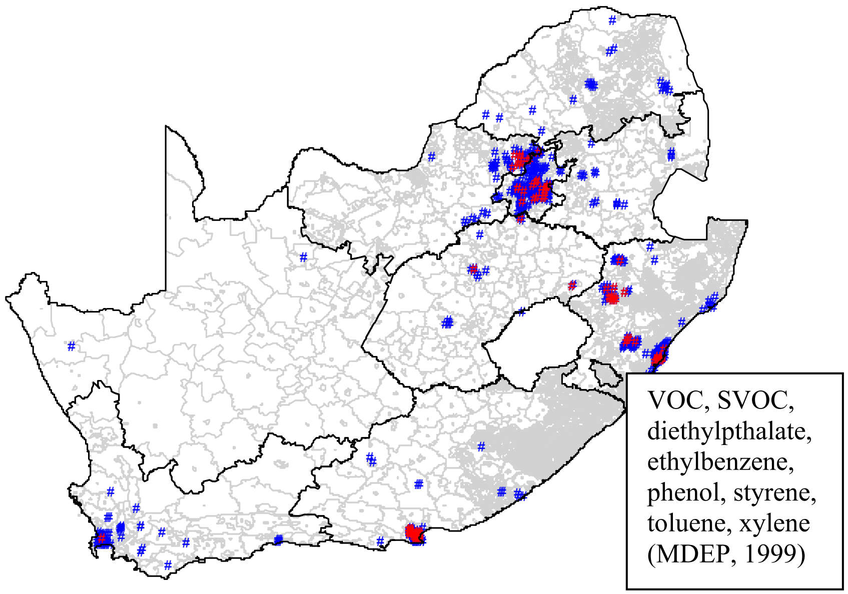
Acetylene, BTEX, Butane, Chloroform, Ethyl Alcohol, Methane, PAHs, Chloroform, CCL4, phenol (WRC, 2004)

Figure 2-17: 335 Production of other chemicals:



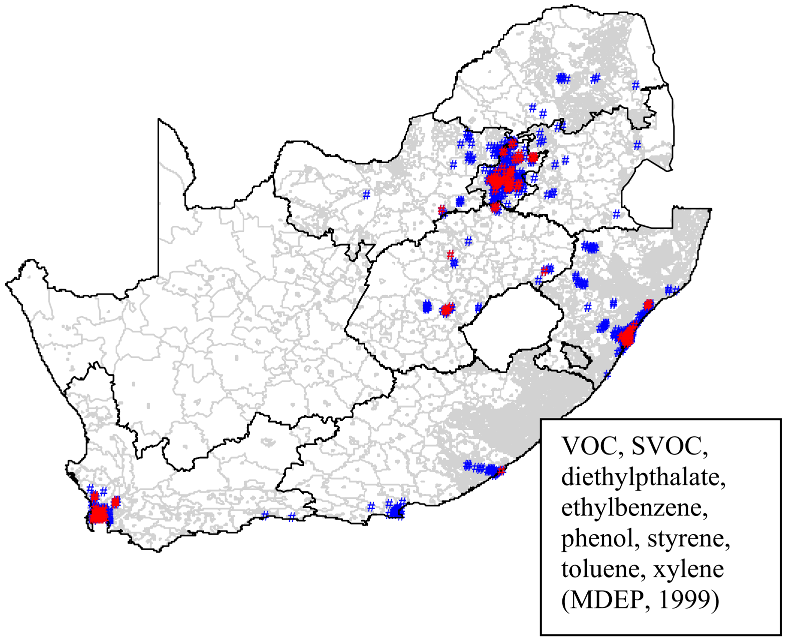
Acetylene, BTEX,
Butane, Chloroform,
Ethyl Alcohol,
Methane, PAHs,
Chloroform, CCL4,
phenol (WRC, 2004)

Figure 2-18: 337 Manufacture of rubber products:



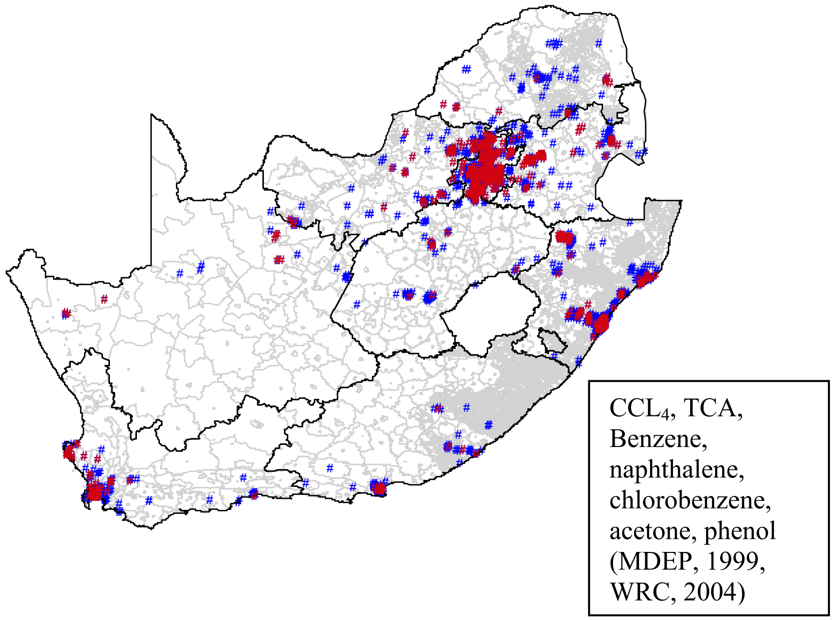
VOC, SVOC,
diethylpthalate,
ethylbenzene,
phenol, styrene,
toluene, xylene
(MDEP, 1999)

Figure 2-19: 338 Manufacturing of plastic:



VOC, SVOC,
diethylpthalate,
ethylbenzene,
phenol, styrene,
toluene, xylene
(MDEP, 1999)

Figure 2-20: 351 Basic Iron and Steel Manufacturing:



CCL_4, TCA,
Benzene,
naphthalene,
chlorobenzene,
acetone, phenol
(MDEP, 1999,
WRC, 2004)

Discussion

The coal and iron mining activities have been plotted on maps to show their relation to the geographic occurrence of their related industries. The collieries (Metalmap, 2001) were also plotted in order to check the correlation of this data with the inferred coal mining areas (from the STATS SA data). The correlation of the collieries – data obtained from Metalmap (2001) - on the map: "Coal Metalmap" and the STATS SA (a), 2001 data - indicating activities directly related to collieries - on the map "210 Coal and Lignite mining", is very high. From this observation it can be concluded that relatively accurate maps can be drawn, using the census data of people active in certain industrial sectors to indicate the specific industries. Iron Ore Mining (241) and the other industrial activities related to steel show only relative correlation. Most steel is transported from the mining areas to larger industrially active areas where the basic steel is further re-worked.

The following conclusions can be drawn from the maps (industrial activities shown in italics, are mines):

Industrial activities covering the largest area of South Africa:

Coal and Lignite Mining, Crude petrol extraction, Fabricated metal, metal services, Food preservation, Manufacture of beverages, Manufacture of Paper and Paper Products, Petroleum Refineries and Synthesizers, Manufacture of Basic Chemicals, Production of other Chemicals, Manufacture of rubber products, Manufacture of plastic, Basic Iron and Steel Manufacturing, Manufacture of structural metal products

Industrial activities with the largest intensity:

Fabricated Metal, Metal Services, Coal and Lignite Mining, Mining of Iron Ore, Food preservation, Manufacture of beverages, Preparation, Spinning and Weaving of Textiles, Manufacture of Paper and Paper Products, Petroleum Refineries and Synthesizers, Manufacture of basic Chemicals, Production of other Chemicals, Manufacture of rubber products, Manufacture of Plastic, Basic Iron and Steel Manufacturing

Industrial activities covering the smallest area of South Africa:

Casting of metals, Iron ore mining, Preparation, spinning and Weaving of Textiles, Dressing and Dyeing of fur, Tanning and Dressing of leather

Industrial activities with the smallest intensity:

Crude petrol extraction and dressing and dyeing of fur.

It can thus be concluded that the industries posing the least risk in terms of intensity (smallest scale and covering the smallest area of South Africa), is industrial activity 315 (dressing and dyeing of fur). The other industries pose a greater risk in that they are either on a large scale or intensity (covering a small area), or they are not as intensive, but cover a large area of South Africa.

The hazard degree of the industries have been included in **TABLE 2-10** below, in which it is aimed to obtain a resultant health risk associated with each industry by linking the chemical risk and the intensity of the industry (on a local scale). The chemical risk has been derived from **TABLE 2-5**, where a small risk is given to industries with a associated total number of polluting chemicals below 11, and high risk is given to a total associated number of polluting chemicals above 11, based on the fact that the median of the values in **TABLE 2-5** is 11.5. The resultant risk has been determined as follows: Large intensity + large chemical risk = Large industrial health risk. The same applies for small intensity and chemical risk, while large intensity and small chemical risk, or vice versa, results in medium industrial health risk.

TABLE 2-10

Industry	**Intensity**	**Risk**	**Resultant industrial health risk**
Metal casting	Large	Large	Large
Structural metals	Large	Large	Large
Fabricated metal	Large	Large	Large
Food preservation	Large	Small	Medium
Beverages production	Large	Small	Medium
Textiles	Large	Small	Medium
Dressing & dyeing of fur	Small	Small	Small
Coal & lignite mine	Large	Small	Medium
Crude petrol extraction	Small	Large	Medium
Iron ore mining	Large	Small	Medium
Tanning & dressing of leather	Large	Large	Large
Paper manufacturing	Large	Small	Medium
Petrol refining	Large	Large	Large
Basic chemicals manufacturing	Large	Large	Large
Other chemicals manufacturing	Large	Large	Large
Rubber manufacturing	Large	Large	Large
Plastic manufacturing	Large	Large	Large
Basic iron steel manufacturing	Large	Small	Medium

2.2 AQUIFER VULNERABILITY

2.2.1 Background information on the compilation of the aquifer vulnerability maps (Parsons, 1998)

The maps used in this study to develop the industrial vulnerability map, have been described in "*Explanatory notes for the Aquifer Classification Map of South Africa*", Parsons and Conrad, 1998:

Three maps were compiled in the 1998 study. The maps are to be used on a regional scale and are not intended for site-specific studies, and such is the industrial vulnerability map as well. The information sources for the aquifer system management classification map are amongst others Vegter (1995) and Reynders (1997). It was not attempted to improve or modify the maps of Vegter and Reynders. The aquifer vulnerability map was compiled using the electronic data of Vegter (1995) and under instruction and supervision of Reynders (1997). Reynders and Lynch (1993) compiled a preliminary vulnerability map for South Africa. For the compilation of the vulnerability map, the DRASTIC model was applied –

Depth to water level	The deeper the water level, the less the chance for the contaminant to reach the groundwater as compared to a shallow water table.
Recharge	The higher the aquifer recharge, the more vulnerable the aquifer will be to contamination.
Aquifer media	This reflects the attenuation characteristics of the aquifer material and reflects the mobility of contaminants through the aquifer.
Soil media	Soils of different types have different water holding capacities and this will influence the travel time of the contaminant. NAPL may adsorb onto soil media.
Topography	High degrees of slope increase runoff and erosion and a gradient in the groundwater heads will also lead to mobilisation of the contaminants.
Impact of vadose zone	This reflects the texture of the soil in the unsaturated zone above the water table.
Hydraulic conductivity	The amount of water percolating to reach the ground water through the aquifer is influenced by the hydraulic conductivity of the soil media.

Each of the parameters was weighted according to relative importance and rating tables presented by Aller *et al* (1987) were modified by Reynders (1997) to accommodate the South African conditions.

The aquifer contamination susceptibility map is simply a product of the aquifer system management classification map and the aquifer vulnerability map. The classes used for each base map were used to develop susceptibility classes. Poor groundwater regions with a low vulnerability are thus defined as having a low susceptibility to contamination. Various parties were consulted as to the appropriateness of the approach used and the categories were then defined and mapped (Parsons, 1995).

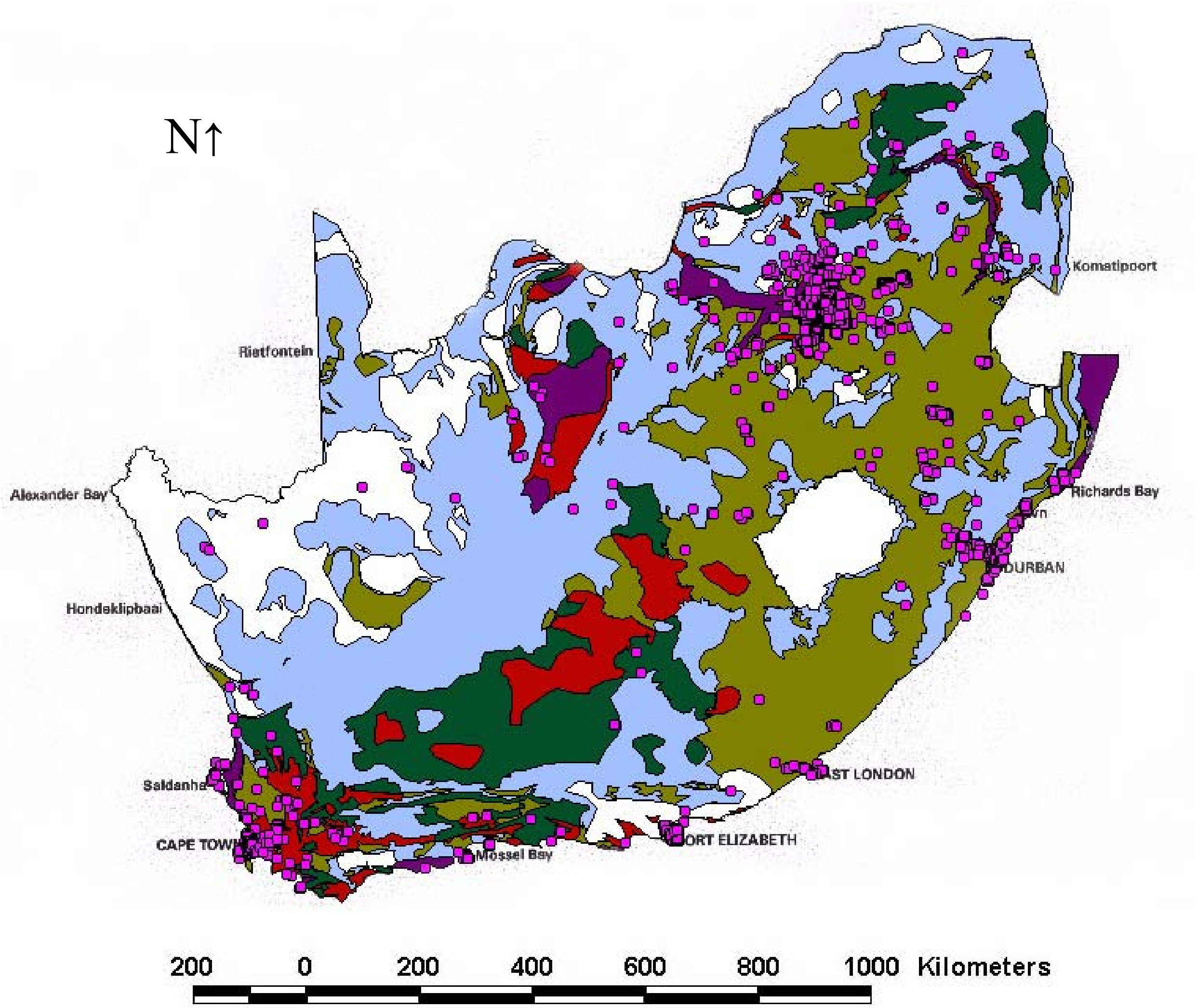
The aquifer contamination susceptibility map was produced by multiplying the reclassified aquifer systems management classification grid with the reclassified aquifer vulnerability grid. This final map has a range of values between 1 and 9 which can be seen in **FIGURE 2-21.**

Important to note is that the aquifer vulnerability map does not take into account industrial activity (Parsons, 1995; Reynders and Lynch, 1993; Parsons and Conrad, 1998), as will be done with the industrial aquifer vulnerability map. A few shortcomings of the DRASTIC classification system in terms of organics are the following: The depth of water level may not play any significant role in the spread and occurrence of NAPL in the aquifer. Dense NAPL will not always follow groundwater flow direction, so the role of topography may be minimized. It should, however, be noted that the vulnerability maps are still largely applicable to organic pollution, despite these shortcomings, and have been used as the basis to work from.

2.2.2 Method of compilation of the Industrial Aquifer Vulnerability Map

The industries were plotted over the Aquifer Contamination Susceptibility Map (called the Industrial aquifer contamination susceptibility map, **FIGURE 2-21**) in order to finally derive the Industrial Aquifer Vulnerability Map. The industries are shown as the purple dots on the aquifer contamination susceptibility map of Parsons, **FIGURE 2-21.** Only the Aquifer Susceptibility Map (Parsons, 1988) was used to compile the Industrial Aquifer Vulnerability Map, since it includes both the Aquifer Classification Map and the Aquifer Vulnerability Map in one map. The Industrial Aquifer Vulnerability Map can be seen in **FIGURE 2-22.**

The largest scale industries (>25 people active per industry) were plotted on the Aquifer Susceptibility Map (signified by the purple dots), where the mentioned map was referenced according to the RSA boundaries.shp file from Metalmap (2001). This gives an indication of the spread of larger industries over the identified vulnerable aquifers of South Africa. It should be noted that a lot of towns are totally reliable on groundwater as a resource, which would constitute a sole source aquifer. These towns were however not plotted since they were not identified in this study, and future research is highly recommended in order to address this question. Sole source aquifers would increase the vulnerability of the town in question to a high degree



Susceptibility Matrix

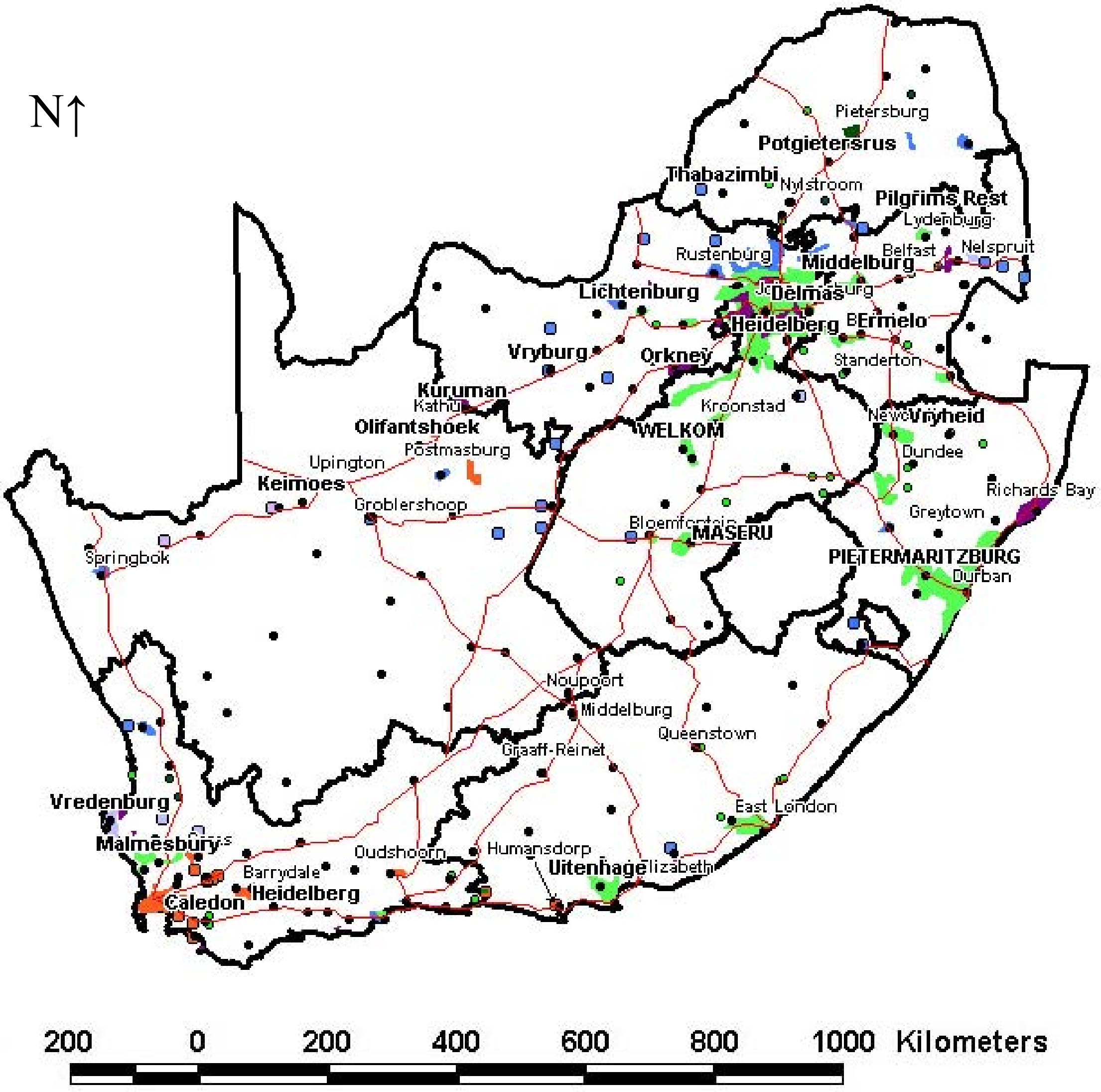
		Aquifer Classification		
		Poor	**Minor**	**Major**
Vulnerability	**Least**	$_{1}$ Low	$_{1}$ Low	$_{3}$ Medium
	Moderate	$_{1}$ Low	$_{4}$ Medium	$_{6}$ High
	Most	$_{3}$ Medium	$_{6}$ High	$_{9}$ High
Legend		●	Industry positions	

Figure 2-21 (Industrial Aquifer Contamination Susceptibility Map)

The aquifer susceptibility map was used in terms of the colour-coding in the susceptibility matrix and on the map, and the industrial vulnerability map was classed as follows:

Colour Code of Aquifer Susceptibility Map	**Aquifer classification and vulnerability description**	**Colour Code of the Industrial Vulnerability Map**	**Description of Industrial Vulnerability Map Code**
White	Aquifer Class: Poor Vulnerability: Least	Lilac	Vulnerability: Very Low
Blue	Aquifer Class: Low Vulnerability: Least AND Aquifer Class: Poor Vulnerability: moderate	Blue	Vulnerability: Low
Olive Green	Aquifer Class: Minor Vulnerability: Moderate	Light Green	Vulnerability: Medium
Dark Green	Aquifer Class: Major Vulnerability: Least AND Aquifer Class: Poor Vulnerability: Most	Dark Green	Vulnerability: Medium to High
Red	Aquifer Class: Minor Vulnerability: Most AND Aquifer Class: Major Vulnerability: Moderate	Orange	Vulnerability: High
Purple	Aquifer Class: Major Vulnerability: Most	Purple	Vulnerability: Very High

The resulting Industrial Aquifer Vulnerability map can be seen in **FIGURE 2-22**.



Industrial aquifer vulnerability map key

Colour Code	Description	Colour Code	Description
🟪	Very low vulnerability	🟩	Medium to high vulnerability
🟦	Low vulnerability	🟧	High vulnerability
🟩	Medium vulnerability	🟪	Very high vulnerability

Figure 2-22 (Industrial Aquifer Vulnerability Map)

2.2.3 Results and conclusions drawn from the Industrial Aquifer Vulnerability map

In the above map, the health risk (see **TABLE 2-10**) has not been included, but will be included below in order to discriminate between high and low hazard industries. From the above map, the following areas can be highlighted according to industry and aquifer vulnerability:

Industrial Areas with very high Industrial Aquifer Vulnerability:

- **Surrounding Johannesburg** (Basic chemicals, other chemicals, paper & beverages production, dyeing of fur, casting of metals, extraction of crude oil, food preservation, iron & Steel manufacturing, Metal Services)
- **Klerksdorp** (Beverages production, Extraction of crude petrol, Food Preservation, Iron & Steel Manufacturing, Metal Services, Petrol refining, Manufacturing of plastic)
- **Orkney** (Steel Products & plastics manufacturing, refining of petrol, metal services, Iron & Steel Manufacturing, Food Preservation)
- **Pretoria** (Casting of metals, Beverages, steel, textiles & other chemicals production, Metal Services, Petrol refining, paper reworking, Basic chemical production, Iron & Steel Manufacturing)
- **Nelspruit** (Food Preservation, Extraction of crude oil, Iron & Steel Manufacturing, Metal Services, Paper production)
- **Richards Bay** (Iron & Steel Manufacturing, Metal Services, Other Chemicals Production, Basic Chemicals Production, Paper Production)
- **Vredenburg, Saldanha (inland)** Casting of Metal, Extraction of Crude Petrol, Food Preservation, Iron & Steel Manufacturing, Metal Services.

Industrial Areas with high Industrial Aquifer Vulnerability:

- **Areas of Johannesburg** (Cast Metal, Beverages, Metal Services, Iron & Steel Manufacturing, Petrol refineries, Paper reworking, Manufacturing of plastic, Basic Chemicals Manufacturing, Other Chemicals Manufacturing)**
- **Newcastle** (Casting of Metal, Food Preservation, Extraction of crude petrol, Metal Services, Iron & Steel Manufacturing, Rubber Manufacturing, Textile Manufacturing)**
- **Durban** (Basic Chemicals, Steel Products, Manufacturing of Plastic, Rubber Manufacturing, Petrol refining, Paper Manufacturing, Metal Services, Iron & Steel Manufacturing, Dyeing of fur, Beverages Production, Extraction of Crude Petrol)**

Port Elizabeth	(Dyeing of fur, Beverages Production, Food Preservation, Extraction of crude petrol, Metal Services, Iron and Steel Manufacturing, Paper Manufacturing, Tanning of leather, Rubber Manufacturing, Textile Production, Other Chemicals Manufacturing)**
Sasolburg	(Petrochemical industries)**
Kroonstad, Virginia, Welkom	(Casting of Metal, Metal Services, Petrol Refining, Rubber Manufacturing)
Carletonville	(Iron & Steel Manufacturing)*
Kathu	(Iron & Steel Manufacturing, Iron Ore Mining)
Postmasburg	(Iron & Steel Manufacturing, Iron Ore Mining)
Oudshoorn	(Tanning of Leather)
Worcerster	(Textiles & Paper Production, Metal Services, Iron & Steel Manufacturing, Food Preservation)
Wellington	(Tanning of leather, Plastic & Paper & Other chemicals production, Iron & Steel Manufacturing, Food Preservation)
Paarl	(Beverages Production, Food preservation, Iron & Steel Manufacturing, Metal Services, production of other chemicals, Paper Manufacturing, Tanning of leather)
Stellenbosch	(Beverages production, Dyeing of fur, Food preservation, Metal Services)

Industrial areas with medium to high Industrial Aquifer Vulnerability:

Polokwane (Pietersburg)	(Dyeing of Fur, Beverages production, Food Preservation, Extraction of crude petrol, Metal Services, Paper Production)
Modimolla (Nylstroom) Area	(Metal Services, Iron & Steel Manufacturing)
Noupoort, Middelburg	(Other chemicals production, tanning of leather)
Humansdorp	(Food Preservation)*

Industrial areas with medium Industrial Aquifer Vulnerability:

Standerton	(Dyeing of fur, food preservation, extraction of crude petrol)
Dundee	(Metal Services)
East London	(Metal Services, Iron and Steel Manufacturing, Manufacturing of Plastic, Basic Chemicals production, Other chemicals production)
Lydenburg	(Iron & Steel Manufacturing)
Queenstown	(Iron & Steel Manufacturing)
Graaff-Reinet	(Food Preservation)*

Industrial areas with low Industrial Aquifer Vulnerability:

- **Springbok**	(Iron & Steel Manufacturing – 4 beneficiation plants - Sishen)
- **Upington**	(Distilleries – wine, and other chemicals)
- **Saldanha** (next to the coast)	(Food preservation, Iron & Steel manufacturing)
- **Robertson**	(Dyeing of fur)*

* Towns originally ranking in a higher industrial aquifer vulnerability area, but with low to medium associated chemical risk. These towns have been moved to a lower rank.

** Towns originally ranking in a lower industrial aquifer vulnerability area, but with a high associated chemical risk. These towns have been moved to a higher rank.

2.3 RESULTS AND CONCLUSIONS

The following can be concluded:

Industries in South Africa that may contribute towards organic pollution:

- Industries other than the petroleum refineries and steel works contribute towards organic pollution of aquifers (Section 2.1.4), which also need to be considered when drafting regulations pertaining to possible polluters. Small-scale industries like paint shops, auto-repair shops etc also contribute towards organic pollution (Section 2.1.6.4).

- Organic chemical production in South Africa is dominated by the production of petroleum-related products (Section 2.1.5). The other 5% is made-up by the production of organic chemicals used in amongst others the cosmetics, pharmaceuticals and food industries. The production of insecticides and herbicides, liquid cosmetics and toiletries and pharmaceutical ointments may have been under-estimated (reasons given in section 2.1.5)

- Possibly 5200 service stations may exist over South Africa that may cause pollution if the underground storage tanks leak (Section 2.1.6.1). Guidelines must be updated or drafted for the installation and monitoring of new underground storage tanks and for the remediation of leaking tanks.

- 16.3 million tonnes of industrial waste is generated per annum, the second highest contribution towards waste after mining. There are currently seven operational hazardous waste sites in South Africa that need to handle the waste generated mostly by industries. Several industries, however, have waste sites that accept only their own waste, and of all these industrial waste-sites only 30 are permitted (Section 2.1.6.2).

- The physical area the industries cover is much larger than originally may have been thought. It would be assumed that only the Durban-Pinetown, Cape Town, Vereeniging-Witwatersrand and Port Elizabeth areas would show industrial activity. Although these show the highest industrial activity that can contribute towards organic pollution, other areas are also highlighted, as can be seen in Section 2.1.7.3.

Industrial activities cover South Africa as follows:

- *Industrial activities covering the largest area:*
  Coal & Lignite Mining, Crude petrol extraction, Fabricated metal, metal services, Food preservation, Manufacture of beverages, Manufacture of Paper & Paper Products, Petroleum Refineries and Synthesizers, Manufacture of Basic Chemicals, Production of other Chemicals, Manufacture of rubber products, Manufacture of plastic, Basic Iron & Steel Manufacturing, Manufacture of structural metal products,

- *Industrial activities with the largest intensity:*
  Fabricated Metal, Metal Services, Coal and Lignite Mining, Mining of Iron Ore, Food preservation, Manufacture of beverages, Preparation, Spinning & Weaving of Textiles, Manufacture of Paper and Paper Products, Petroleum Refineries and Synthesizers, Manufacture of basic Chemicals, Production of other Chemicals, Manufacture of rubber products, Manufacture of Plastic, Basic Iron and Steel Manufacturing

The risk associated with the different industrial activities is as follows:

“Risk” is defined in this sense as (a) chemical risk (which is the amount of chemicals (which may be carcinogenic or non-carcinogenic and/or toxic or non-toxic) that are associated with an industry which may cause a harmful effect to human health) in association with (b) the intensity of risk (which is associated with the scale of the industry), and (c) with the aquifer vulnerability, e.g. “Is it overlying an aquifer vulnerable area?”). Risks (a) and (c) coupled give the associated industrial health risk. Least risk thus signifies an industry with the lowest probability of causing a harmful effect while highest risk indicates the opposite.

- Industries posing the highest risk are: Metal casting, structural metals manufacturing, fabricated metal manufacturing, tanning and dressing of leather, petrol refining, basic chemicals manufacturing and rubber and plastics manufacturing.

- The industry that poses the lowest risk is: Dressing and dyeing of fur.

Aquifer vulnerability:

Aquifer vulnerability relates to industrial activities overlying aquifer vulnerable areas. This vulnerability has been coupled with chemical risk associated with each industry in order to derive high risk to low risk towns, which are shown in Section 2.2.3.

Chapter 3

Legislation

3.1 SOUTH AFRICAN REGULATORY FRAMEWORK

Environmental law is a new, distinct branch of law. This body of law is extremely wide, and the scope imprecise. (Rabie, as cited by Glazewski, 2000). This is still the case in 2005 – only three new principal laws related to the environment have been proposed since 2000 - The South African Weather Services Act (No. 8 of 2001), the Protected Areas Act (No. 57 of 2003), and the Biodiversity Act (No. 10 of 2004), none of which are related to organic pollution. A proposal to regulate filling stations under the National Environmental Management Act (NEMA) is first being considered in Notice No. 12 of 2005 in the GG 27163 of 14 January 2005. This is a cause for concern for most environmental law practitioners and implementers of the law (government bodies) in South Africa.

Several acts exist in South Africa pertaining to waste management, actions to be taken against potential polluters, as well as remedial action. The National Water Act (NWA) requires site remediation, but very little regulatory guidelines exist on how this can be attained. Little guidance exists on the processes that must be followed to get from the stage where the problem is identified up to the point of remediation. The task is made more difficult by the fact that all the laws of the different departments must be harmonized in such a way that all the legal implications of a decision are considered so as to prevent illegal processes from occurring. Regulations should drive cleanups and hence site characterization at polluted and hazardous waste sites and it is thus imperative that South Africa develops guidelines for site characterization for different types of pollution.

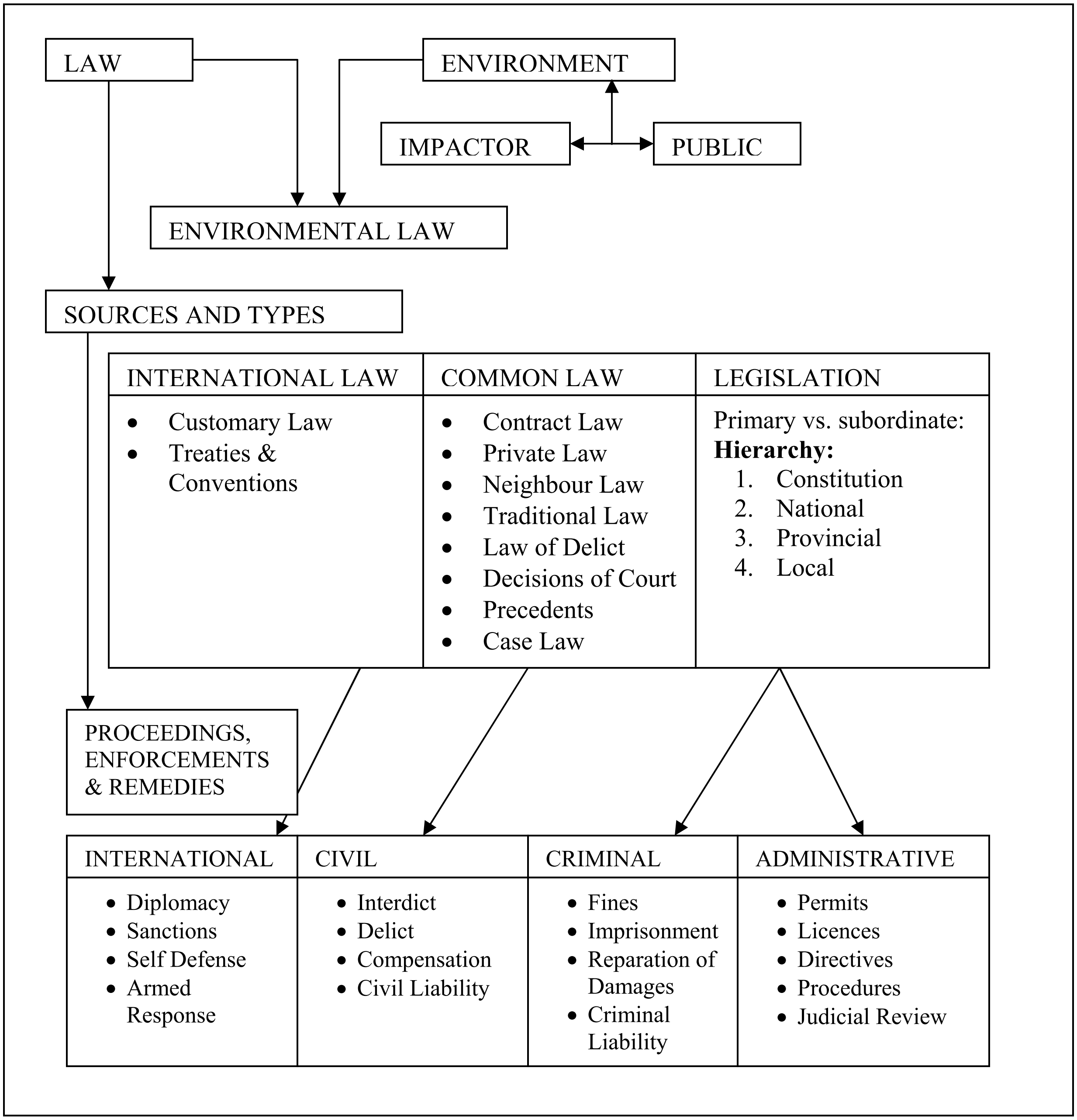
A few definitions will be listed below before proceeding to the different acts that exist in South Africa:

Accession – A term used to coin the action of a state or country becoming party to a treaty in whose negotiation it did not participate, and which it did not sign. Multilateral law-making treaties that seek to achieve a large measure of universality include an accession clause. (Dugard, 2000) Accession has the same legal effect as ratification. However, unlike ratification, which must be preceded by signature to create binding legal obligations under international law, accession requires only one step, namely, the deposit of an instrument of accession. (United Nations, 2003)
Regulation – Describes the manner in which sections in acts must be abided by.
Policy – A rule or regulation promulgated, adopted, or ratified by the governmental entity's legislative body (LLLL, 2003) (the paper foregoing the “Green Paper”)
Ratification (of treaties) – Formal international agreements like treaties (conventions) have to be ratified if treaties indicate a requirement for ratification, this binds the partaking country to implementing the treaty in the form of legislation in the concerned country (Dugard, 2000).

Sanction - That part of a law, which inflicts a penalty for its violation, or bestows a reward for its observance. Sanctions are of two kinds, those that redress civil injuries, called civil sanctions; and those, that punish crimes, called penal sanctions (LLLL, 2003).

Signature (of treaties) – At a conference of plenipotentiaries, a state will sign an agreed text. No legal obligation is imopsed, but an obligation of good faith in refraining from acts calculated to frustrate the object of a treaty until such time as the party decides to ratify or makes it clear that it does not want to become party to a treaty (Glazewski, 2000).

The environmental law and proceedings and remedies as practiced in South Africa, are set out in **FIGURE 3-1** (DWAF, 2001)



The different primary sources of environmental law are international law and the South African law (which is sub divided into common law and legislation). The sources and remedies will be described in more detail in sections 3.1.1 to 3.1.2.

3.1.1 International law

International concern about growing pollution has escalated over the past 20 years. This is evident in the large amount of protocols and conventions that have arisen (see more about protocols ratified by South Africa in section 3.3), as well as countless reports and conferences on integrated waste management and sustainable use of resources. Sources of international law are customary law (generally accepted practices of states that were established over a long period of time), also called 'soft law' (Dugard, 2000) and treaties and conventions (agreements between states, recent as well as long-standing, which is signed by all participating countries), also called 'hard law' (Dugard, 2000). Soft law is part of a deliberate cooperative strategy and makes no attempt to employ the language of obligation found in treaties, thus soft law instruments are not enforceable. South Africa extensively implements Agenda 21 and subscribes to the Rio Declaration, a convention that arose from The Rio Earth Summit in 1992.

South Africa is party to over 50 international treaties, directly or indirectly relevant to the environment. (Glazewski, 2000). According to the "*Integrated pollution and waste management for South Africa"* policy, there are 26 international agreements (17 conventions, 4 protocols, 3 treaties and 2 agreements) that pertain to integrated pollution and waste management. Nineteen of these have been acceded to or ratified by South Africa. In section 3.3 treaties ratified by South Africa, pertaining to NAPL pollution, are described.

3.1.2 South African law

Two types of law exist, which are common law and legislation.

- **Common law (also precedents and traditional law)**

Common law applies when a matter is not governed by legislation. The South African Common Law is based on the Roman Dutch Law, but was also influenced by the English Law and Traditional Law.

Sources of common law are for instance: Contract Law, Law of Delict, Property Law, Private law, Court decisions establishing precedents, Procedural Law (especially civil proceedings – e.g. interdict), Neighbour law etc. The *Law of Nuisance ("burereg")* is important as a source of environmental law, since it regulates conduct by which a neighbour's health or well-being in the occupation of his or her land is interfered with, as well as damage to his or her property (DWAF, 2001).

- **Legislation**

When applying legislation, it must be determined which legislation has the authority to overrule the other. A distinction must be made between original (primary) legislation and subordinate legislation. Original (primary) legislation pertains to Acts of Parliament, as well as laws made by any of the nine Provinces (DWAF, 2001). Subordinate legislation derives its authority from primary legislation. This includes regulations, ordinances, proclamations and authorizations such as licenses, general authorizations, permits and even policy (DWAF, 2001).

A listing of the legislation in South Africa in their relative statutory importance are given as follows:

1. Constitution
2. Parliamentary or National Legislation (Acts of parliament) – (National Environmental Management Act - NEMA, National Water Act - NWA, Water Services Act - WSA)
    i. Provincial Legislation
    ii. Laws from 1994
    iii. Proclamations between 1986-1994
3. Ordinances before 1986
4. Local authority bylaws

This means that the Constitution is the only legislation that has the authority over the NEMA and NWA, and these acts have authority over provincial laws.

3.1.2 Provincial and private laws

Several provincial and private laws may exist regarding water and NAPL pollution, but these laws are not applicable nationally and will thus not be focused on in this chapter.

3.2 SOUTH AFRICAN STATUTES PERTAINING TO ORGANIC POLLUTION

A short summary of the different South African statutes pertaining to water resource pollution (and indirectly NAPL pollution) will be described in this section. Any shortcomings and useful legislation will be highlighted.

The Constitution - 1997

The Constitution describes the general right of every citizen of South Africa to an environment that is not harmful to their health and well-being and that is protected for future generations (Section 24).

> Good law enforcement can be practiced by following international example, i.e. by abiding by international law through the ratification of treaties (see Section 3.3) and writing those treaties into South African legislation.

The National Water Act (NWA) - 1998

The National Water Act (1998) describes the protection of water resources (Chapter 3). Part 4: section 19 of chapter 3 deals with measures to be implemented in case of pollution occurrences. Part 5 deals with emergency incidences, and a shortcoming that has been observed here, is the following:

> The guidelines for the clean-up procedures and remedying the effects of the incident must be written and regulations drafted in order to ensure uniform application in South Africa. *At this stage each province has its own way of handling spills and each Fire Department also can only serve certain areas in a radius around a city* (Free State Fire Dept, 2003). Large stretches of road are unattended (for instance along the N1 where small towns do not have Fire Departments). It is estimated that 90% of trucks on South African roads carry hazardous chemicals, mixed with more conventional loads like furniture (DEAT (c), 2003) and law enforcement with regard to this transportation is inadequate.

Chapter 4 (Part 1, Section 21) lists the different permissible water-uses, that are to be registered and licensed with the Department of Water Affairs and Forestry (DWAF). In order to manage water usage, the Minister may make regulations under section 26 (1).

> This section of the Act is enabling and it is recommended that specific regulations be written with regard to NAPL management in South Africa.

Chapter 4, Part 5, section 37 allows the minister to regulate activities having a detrimental impact on water resources by declaring them controlled activities. Four such activities have been listed, and section 37 (e) lists *an activity, which has been declared as such under Section 38.*

> The production of NAPL wastes as by-products of industrial processes can be declared a controlled activity, but it is envisaged that writing regulations under the NWA may address the NAPL pollution problem more effectively.

In common with other Acts of Parliament, which aim to make non-compliance a criminal offence, Chapter 16 lists the acts and omissions, which are offences under the NWA, with the associated penalties.

> Chapter 16 gives the courts and water management institutions certain powers associated with prosecutions for these offences.

The National Environmental Management Act (NEMA) - 1999:

Chapter 6 (Section 25(1)) of the NEMA states that the Minister may make a recommendation to Cabinet and Parliament regarding accession to and the ratification of an international environmental instrument, where the Republic is not yet bound by an international environmental instrument.

> This provision in the Act can be used with success to regulate NAPL problems with international law where management principles have not yet been established in South Africa.

Section 28 (1) imposes duty of care upon all polluters and (2) stipulates responsible persons on whom this duty is imposed. Section 30 describes how emergency incidents are to be controlled. Subsection 1 lays down definitions in terms of emergency incidents and Subsection 2 authorizes a relevant authority to take steps. The steps may only be taken by the *Director General of a Department if no steps have been taken by lower hierarchy authorities mentioned in the previous sections*.

> This negative obligation on authorities from refraining to take action is difficult to understand. In practice it is difficult to identify responsible authorities and it should rather be made clear whose responsibility what is.

According to Section 46, the Minister may make model bylaws aimed at establishing measures for the management of environmental impacts of any development within the jurisdiction of a municipality, which may be adopted by a municipality as municipal bylaws.

> This part of the Act enables the Minister to write regulations regarding the handling of NAPLs, which could assist municipalities to attend to the impacts associated with NAPL's on a local but uniform level.

The Environment Conservation Act (ECA) - 1989:

Part V, Section 21 makes provision for the identification of activities, which may have a substantial detrimental effect on the environment.

> Of particular importance for NAPL pollution, are the following activities listed under subsection (2): (b) water use and disposal, (f) industrial processes, (g) transportation, (i) waste and sewage disposal and (j) chemical treatment. According to subsection (3) the Minister may identify an activity in terms of subsection (1) after consultation with relevant and competent ministers or authorities. Disposing of NAPL-containing waste(water) - (for instance in the form of car-wash detergent runoff) may be identified as a detrimental activity.

According to Part VI, Section 24, the Minister of Department of Environmental Affairs and Tourism (DEAT) can make regulations regarding waste management.

The provision of regulations that can be made with regard to the classification of different types of waste and the handling, storage, transport and disposal of such waste in Subsection (c) can be used to address NAPL pollution problems.

3.3 TREATIES AND CONVENTIONS PERTAINING TO ORGANIC POLLUTION

Information pertaining to the treaties and conventions (International Law), covering pollution (by organics) that South Africa ascribes to are listed below:

Basel Convention (Convention on the control of transboundary movements of hazardous wastes and their Disposal)
Rotterdam Convention (Convention on prior informed consent)
Stockholm Convention on Persistent Organic Pollutants

Note: Several treaties exist for pollution of the sea by oils (e.g. The London Convention). These are not described since the scope of the thesis concentrates on organic pollution on land. The Antarctic Treaties also covers oil pollution on Antarctica but this is not relevant in South Africa. It can however, be adopted in South African law in order to control NAPL pollution.

3.3.1 Detail on conventions related to water and NAPL pollution

Basel Convention (Convention on the Control of Transboundary Movements of Hazardous Wastes and Their Disposal) – DEAT (a), 2004

Acceded:	April 1994
Ratified:	May 1994

The main objectives of the Convention are the *reduction of the production* of hazardous waste and the *restriction of transboundary movement and disposal* of such waste. It also aims to ensure that any transboundary movement and disposal of hazardous waste (including NAPL containing waste), when allowed, is strictly controlled and takes place in an environmentally sound and responsible way. Locally, the Waste Management Bill is under preparation, and this bill will enact the Basel Convention.

Improved international cooperation has resulted in better control of hazardous waste movements and complete transparency in cases where such movements do occur. The ban on hazardous waste movements from OECD (Organization for Economic Co-operation and Development) countries to non-OECD countries for final disposal and recycling came into effect in 1998, but has not been ratified by a sufficient number of parties yet.

Rotterdam Convention (Convention on Prior Informed Consent) – DEAT (b), 2004
Acceded: 2002

The Convention represents an important step towards ensuring the protection of citizens and the environment in all countries from the possible dangers resulting from trade in highly dangerous pesticides and chemicals. The convention will enable the world to monitor and control the trade in very dangerous substances. It will give importing countries the power to decide which chemicals they want to receive and to exclude those they cannot manage safely.

The convention ensures obligatory detailed information exchange between countries on hazardous chemicals and pesticides allowing informed decision-making on the national use of such chemicals. Chemicals controlled include: Pesticides: 2,4,5-T, aldrin, captafol, chlorobenzilate, chlordane, chlordimeform, Dichloro-diphenyl-trichloroethane (DDT), dieldrin, dinoseb, 1,2-dibromoethane (EDB), fluoroacetamide, HCH, heptachlor, hexachlorobenzene, lindane, mercury compounds, pentachlorophenol and certain formulations of methyl-parathion, methamidophos, monocrotophos, parathion, phosphamidon. Industrial chemicals: crocidolite, polybrominated biphenyls (PBB), polychlorinated biphenyls (PCB), polychlorinated terphenyls (PCT), tris (2,3 dibromopropyl) phosphate.

Stockholm Convention on Persistent Organic Pollutants (DEAT (c), 2004)
Ratified: 2001
Acceded: 2002

The objective of the Convention is to protect human health and the environment from the effects of chemical pollutants commonly known as persistent organic pollutants (POPs). Twelve persistent organic pollutants (POPs) have been targeted for immediate action and discontinuation of use. The 12 selected chemicals are: aldrin, chlordane, DDT, dieldrin, endrin, heptachlor, hexachlorobenzene, mirex, toxaphene, PCBs, dioxins and furans. South Africa applied for an exemption for the use of PCBs in transformers and DDT for pest control until an effective alternative has been found.

3.3.2 The status of the conventions in South African legislation

South Africa has ratified the Stockholm and Rotterdam conventions. These two conventions will only enter into force after the submission of the 50th instrument of ratification, meaning at least 50 countries must sign the convention before it is enforced. South Africa, can, however, in the meantime, start with plans of incorporating these instruments into our environmental management system. None of these treaties have been incorporated as yet into South Africa's legislative system. The Basel Convention has been ratified. It entered into force in 1992. The provisions of this convention are being taken into account in the development of the Waste Management Bill, which is still in its early stages (DEAT Personal Comm., 2003).

Important to note, is that South Africa can convert the treaties (and international law) to South African legislation in order to effectively control NAPL pollution. A large amount of NAPL-related treaties may exist that can also be ratified to.

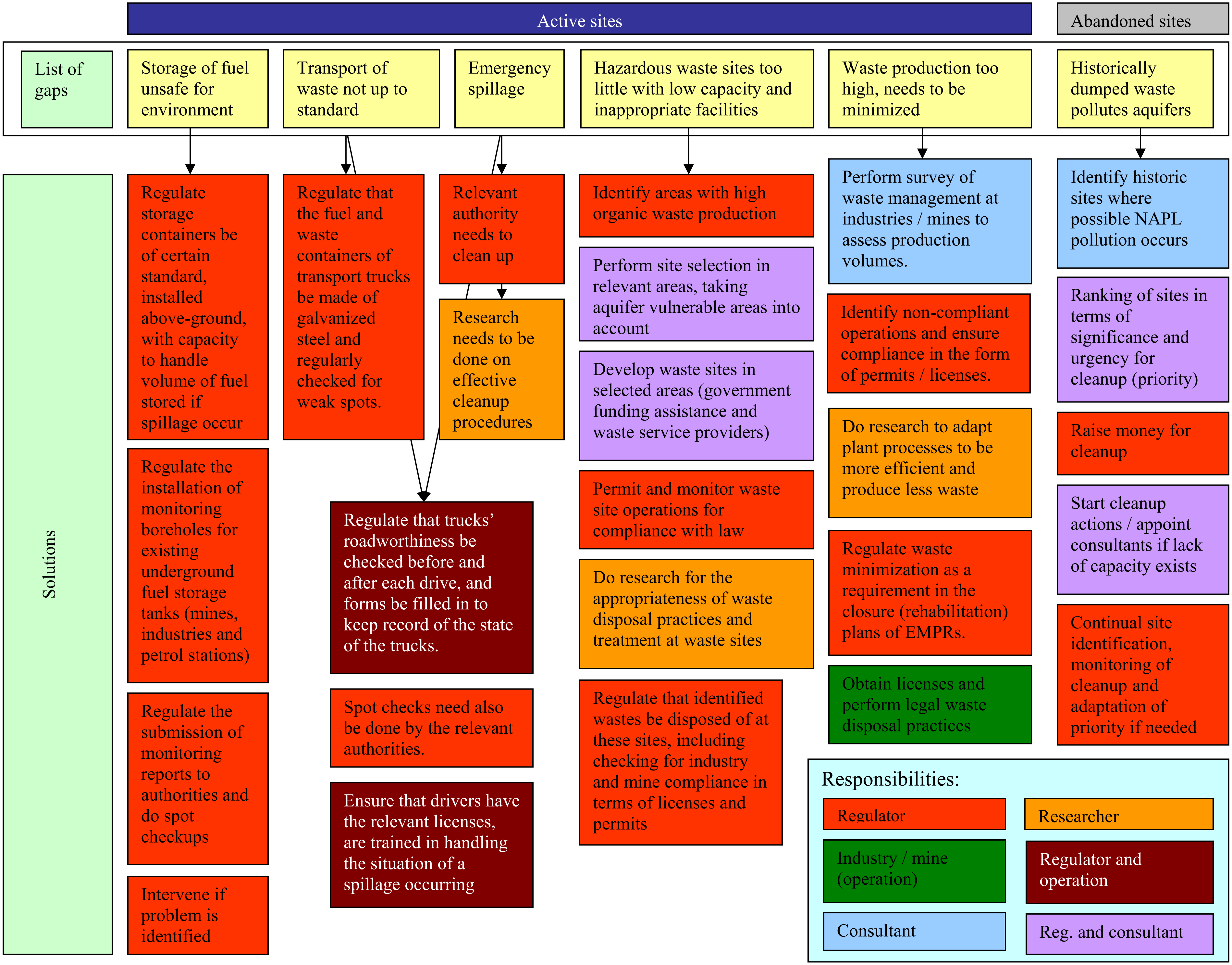
3.4 REGULATIONS THAT ARE NEEDED TO ADDRESS ORGANIC POLLUTION

"South Africa has at its disposal a plethora of environmental laws and statutory provisions. Given this sophisticated armoury of legislative weaponry, the question arises as to why environmental degradation continues apace." (Glazewski, 2000, p143). The answer to this question probably lies in the implementation of the laws. This section does not aim to give answers to this difficult question, but rather aims to recommend the development of certain regulations that may be of use in addressing the NAPL problem. Shortcomings that need to be addressed in order to better handle the NAPL pollution problem, are listed below.

- Define responsible authority that is to take action and define the action to be taken for emergency response for NAPL and other hazardous chemicals spills – (Section 30, NEMA; NWA, Chapter 3, part 5, as well as White Paper on Disaster Management). According to DEAT (c) (2003), emergency response plans for chemicals spills are adequate, but there is limited capacity for their implementation, monitoring and enforcement. According to Glazewski (2000) the NEMA places a negative obligation on authorities from refraining to take action, which is difficult to understand. In practice it is already difficult to identify responsible authorities and it should rather be made clear whose responsibility what is.
- Interim action measures for sites with ongoing NAPL release.
- Cleanup measures (remediation) or the inactivation of pollution (adapted to the South African situation) from long term NAPL pollution sites.
- A process (action plan) to be followed when addressing LNAPL and DNAPL pollution sites (specifying distinctive roles for regulators, consultants and the polluter).
- Regulations on the investigation procedures for NAPL, e.g. invasive and non-invasive, drilling and sampling of NAPL.
- Regulations on ensuring the safety of site investigation personnel (drillers and samplers).
- Regulations on the transfer of NAPL waste, as well as disposal of the different types of waste.
- Regulations on the requirements for the building of the underground storage tanks.
- Making the ongoing ground water monitoring and report of fuel station spillages to the relevant authorities obligatory. This is needed in order to identify possible pollution at early stages in order to stop pollution and remediate the site (remediation of Light NAPL is more attainable that Dense NAPL). All measures should be taken to minimize and remediate all possible pollution, thus the same is required for heavy and light industries that may contribute towards organic pollution.
- Regulations for small-scale industries (a cleaning protocol for e.g. paint shops, service stations etc.) that ensure that these do not pollute the environment when it can be avoided.

- The phasing out of the use of certain persistent organic pollutants and replacing them with more environmentally friendly chemicals.
- Making the use of chain of custody forms obligatory for all sectors in the case of a investigation – Industry, Consultants, Laboratories and Regulators.
- Policies to control waste disposal are inadequate (CAIA, 2002 and DEAT (c), 2003).
- Legislation relating to exposure limits from chemical production is outdated (air pollutant emissions dioxins, furans – (CAIA, 2002 and DEAT (c), 2003).
- No tracking or audit system for chemicals – customs and excise staff (CAIA, 2002).
- Material safety data sheets are designed for industry and not user friendly – need update
- Incompatibility of chemicals is not considered and the synergistic effect of chemicals not investigated and reflected in material safety data sheets (MSDS's) (CAIA, 2002).
- Disposal of toxic chemicals in South Africa is not necessarily reflected and stock piling of waste occurs (Stakeholder workshop, June 2002)
- The practice of risk assessment applied to the production and use of chemicals has been lacking in South Africa. Toxicity testing does not take into account the synergistic effect of combining chemicals. (CAIA, 2002)
- Lack of laboratory skills in South Africa with only a few accredited laboratories. Skills audit on labs is lacking in SA. (CAIA, 2002)
- The requirements of the Basel Convention in terms of minimization of waste production still need to be incorporated in SA legislation. Greater clarity is needed on the definition of hazardous and toxic chemicals. (CAIA, 2002)
- No coherent approach to the rehabilitation and registration of contaminated sites exist. A national inventory of the location of contaminated sites has not been undertaken. There is currently no fund (national of private) for the closure and rehabilitation of industrial of sites.

A flow chart that identifies the main problems that need to be addressed at active and abandoned industrial and mining sites, as well as the possible solutions and whose responsibility each action is, can be seen below. All the regulations that need to be drafted, are not listed in this flow chart.



Active sites

Abandoned sites

List of gaps

Storage of fuel unsafe for environment

Transport of waste not up to standard

Emergency spillage

Hazardous waste sites too little with low capacity and inappropriate facilities

Waste production too high, needs to be minimized

Historically dumped waste pollutes aquifers

Solutions

Regulate storage containers be of certain standard, installed above-ground, with capacity to handle volume of fuel stored if spillage occur

Regulate the installation of monitoring boreholes for existing underground fuel storage tanks (mines, industries and petrol stations)

Regulate the submission of monitoring reports to authorities and do spot checkups

Intervene if problem is identified

Regulate that the fuel and waste containers of transport trucks be made of galvanized steel and regularly checked for weak spots.

Relevant authority needs to clean up

Research needs to be done on effective cleanup procedures

Regulate that trucks' roadworthiness be checked before and after each drive, and forms be filled in to keep record of the state of the trucks.

Spot checks need also be done by the relevant authorities.

Ensure that drivers have the relevant licenses, are trained in handling the situation of a spillage occurring

Identify areas with high organic waste production

Perform site selection in relevant areas, taking aquifer vulnerable areas into account

Develop waste sites in selected areas (government funding assistance and waste service providers)

Permit and monitor waste site operations for compliance with law

Do research for the appropriateness of waste disposal practices and treatment at waste sites

Regulate that identified wastes be disposed of at these sites, including checking for industry and mine compliance in terms of licenses and permits

Perform survey of waste management at industries / mines to assess production volumes.

Identify non-compliant operations and ensure compliance in the form of permits / licenses.

Do research to adapt plant processes to be more efficient and produce less waste

Regulate waste minimization as a requirement in the closure (rehabilitation) plans of EMPRs.

Obtain licenses and perform legal waste disposal practices

Identify historic sites where possible NAPL pollution occurs

Ranking of sites in terms of significance and urgency for cleanup (priority)

Raise money for cleanup

Start cleanup actions / appoint consultants if lack of capacity exists

Continual site identification, monitoring of cleanup and adaptation of priority if needed

Responsibilities:

Regulator

Researcher

Industry / mine (operation)

Regulator and operation

Consultant

Reg. and consultant

3.5 CONCLUSIONS AND RECOMMENDATIONS

The following remarks are relevant:

- Proper definitions to determine legally whether an industry is compliant under the existing legislation exist, but no specific guidelines regulating NAPL could be found in the legislation.
- The International Conventions must be included in and enforced by National Law. Currently DEAT is in the process of including the Basil Convention in the NEMA, which will regulate transboundary movement of NAPL waste. Regulations will have to be made on the reduction of production of hazardous waste. This may entail the research and development of safer environmentally friendly plant processes by industrial process engineers. Research is also needed to enforce the Stockholm convention. Currently PCBs and DDT (persistent organic pollutants) are still used in South Africa and alternative safer and effective chemicals have to be found.
- The regulations must be updated to sufficiently address the problem of disposal, handling and storage of chemicals. Regulations can be the following:
  - Ensuring that diesel and petrol pollution occurrences are minimized on mining and industrial sites by requiring that the tanks *only* be installed above-ground, with a spillage capturing pit that can handle the volume of fuel kept in the tank, should the tank develop a leak.
  - Ensuring that areas where machinery and trucks of mines and industries receive fuel, are lined with a concrete slab and have a drainage system that can handle fuel spillage, where this waste water has to be disposed of at hazardous waste sites or treated.
  - Ensuring that (a) enough hazardous waste sites exist that (b) have the capacity to receive wastes and (c) can appropriately dispose of or treat the waste. Alternatively waste production can be minimized by requiring that industries and mines allocate part of their income, in association with funding from government, to research and development of more environmentally friendly production processes. Similar regulations that require reduction of waste with the plan on rehabilitation cost savings can also be included in the mine closure plans for Environmental Management Programme Reports (EMPRs).
  - Ensuring that trucks carrying waste to these waste sites are up to standard to handle the type of waste carried and ensuring that the drivers of these trucks know how to handle the possibility of a spillage (i.e. to report it to the local Fire Department and DWAF for immediate cleanup action).
- Plans must be developed for addressing historical NAPL release problems.
- Historical waste (dump) sites at abandoned sites need to be identified and the pollution needs to be addressed.
- The different government departments need to streamline their processes in order to cut out unnecessary work, finish permitting procedures faster and prevent the illegal duplication of permitting disposal sites. One example of such an illegal process is when the Department of Water Affairs gives a waste site a license under the NWA and the Department of Environmental Affairs gives the same

site a permit under the NEMA. This site must be regulated by either the water use license or the waste site permit, but not both.

Chapter 4

NAPL physical properties and other parameters required

4.1 BACKGROUND

Chapters 5 and 6 will focus on Site Assessment and Characterization. To understand the proposed methodologies, it is important to discuss the physical, hydraulic and chemical properties of NAPL's.

The determination of NAPL properties is of paramount importance during the Site Characterization and the Remediation phases, to identify such factors as migration and stability. When certain properties like wettability, density and viscosity have been determined, the conceptual model can be refined and ultimately a remediation option can be chosen for the specific NAPL and the geology in which it is located. Determining the NAPL properties will, for instance, aid in site characterization by getting an idea of whether the NAPL will migrate far from the source and whether it has been degraded substantially or not (which is important for the deciding on exercising remediation and the selection of a remediation option). The NAPL characteristics will also have an effect on aquifer vulnerability. Hard rock aquifers will be much more vulnerable to DNAPL pollution than porous aquifers. The DNAPL pollutant constantly searches the most effective pathway, which are fractures in hard rock. Much larger aquifer systems can be polluted in this way and remediation thereof is almost impossible.

In this section, different properties of NAPL and the determination thereof, will be listed. The practicability and limitations of exercising certain options in South Africa will also be described. **APPENDIX A** (on CD) lists certain NAPL organic chemicals' properties that can be used to determine certain unknown properties of organic chemicals (e.g. Kd values, effective solubility etc.), given certain parameters.

The following notes in relation to **APPENDIX A** (included on CD) are important:

- The chemicals are given and listed alphabetically under two separate sections: volatile organic compounds (VOC's) – Data Set 1; and semi-volatile organic compounds (SVOC's) – Data Set 2.
- LNAPL chemicals are highlighted in dark grey.
- A reference number is given for each value, of which the reference information can be found at the end of each section.
- Some log Koc (organic carbon partition coefficient) values that could not be found in literature were calculated using the following equation: $\log (K_{oc}) = 0.830 \log (K_{ow}) + 0.3$ by Matthes *et al*, 1985 (as cited by Spitz and Moreno, 1996). In the case where the log (Koc values were calculated, the reference will be cited as follows: Est (estimated) from Kow (octanol water partition coefficient).

- The Henry's Law constant values are given as atm-m3/mol units, but values shown as italics, are given as Pa-*m*^{3}*/g mol* units.
- A row has been included in the data sets, which show if the Kd (distribution coefficient) value is determinable, using the equation Kd = Koc × foc.
  - If value = 0;	Kd is not determinable.
  - If value = 1;	Kd is determinable using the above equation.
- Abbreviations:
  N/R = Not Reported

The parameters listed in **APPENDIX A** can be used to form the conceptual model. Several uses are listed in Section 6.6 in Chapter 6, and these parameters are applied in Chapters 7 and 8.

One example will be given to illustrate the use of the parameters given in **APPENDIX A**.

The foc-value for the soil has been determined as 0.001 by a laboratory analysis of a soil sample obtained from the investigated site. The koc-value for benzene has been determined as 87.78 L/kg by a laboratory. Since benzene is a non-polar organic chemical, the Kd-value can be determined by the equation Kd = koc × foc. This gives a Kd-value of 0.08778 L/kg. This Kd value can be used to determine the retardation factor (Rf), which expresses the rate of movement of the contaminant versus the rate of movement of the water and is determined by the following equation: $Rf = 1 + \frac{K_d \rho}{n}$ (Environment Agency, 1999), where ρ is the bulk density (g/cm3) and n is the effective porosity. Assuming that the bulk density is 1.6 g/cm^3 and the effective porosity is 0.02, the retardation factor will be 8.0224. The retardation factor expresses how much slower a contaminant moves compared to the groundwater. Higher soil organic carbon content increases the retardation factor. The retardation factor is generally proportional to the degree of hydrophobicity of the compound (expressed by the octanol/water partition coefficient – the Kow) (Pankow and Cherry, 1996). The more hydrophobic the organic compound is, the more it will be retarded, while a contaminant like Cl is not retarded and is viewed as a conservative (non-reactive) chemical.

4.2 PROPERTIES OF DNAPL VS LNAPL

The difference in properties between Dense Non-Aqueous Phase Liquid (DNAPL) and Light Non-Aqueous Phase Liquid (LNAPL) is given in the **TABLE 4-1**. The difference between the two types of pollutants plays a significant role in their migration and ultimately in the possibility for remediation. The fact that LNAPL is less dense than water means that deep aquifer contamination is less likely than with DNAPL. LNAPL is also more readily remediated than DNAPL (it can be removed from the water by bio-skimming, for instance). The lower viscosity of DNAPL does, however, imply lower migration rates than for LNAPL.

TABLE 4-1: Properties of DNAPL vs. LNAPL		
Property	**DNAPL**	**LNAPL**
Density	More dense than water [1]	Less dense than water [1]
Viscosity	Usually more viscous than water [2], except chlorinated hydrocarbons [3]	Usually less viscous than water [2]
Saturation (residual)*	0.75 - 1.25% (light oil in highly permeable media) 20% (heavy oil)[3]	10-20% (Unsaturated Zone) 15-50% (Saturated Zone)[4]

1. Pankow and Cherry, 1996; 2. Bromhal *et al,* 2003; 3. Huling and Weaver, 1991, 4. Mercer and Cohen, 1990
* Residual saturation is defined as the volume of hydrocarbon trapped in pores relative to the total volume of pores (Huling and Weaver, 1991)

4.3 NAPL PHYSICAL PARAMETERS AND DETERMINATION

The physical parameters (related to NAPL) that are required for performing a site assessment and characterization will be described below. The use of each parameter in the determination of other parameters will be highlighted. Non-NAPL related physical parameters that need be determined will also be described.

4.3.1 Density (ρ)

Density (ρ), usually measured in kg/m^3 is the mass per unit volume of a substance. It is often presented as specific gravity (S.G.), the ratio of a substance's density to that of some standard substance (usually water) at a specified temperature. Density varies as a function of several parameters, and most notably temperature (Cohen and Mercer, 1993). If a NAPL has an S.G. less than water, generally less than 1.0, it is less dense than water (i.e., LNAPL) and will float on water. If it has an S.G. greater than water, generally greater than 1.0, it is denser than water (DNAPL). The density of most fluids generally decreases as temperature increases. Consequently, the density of fluids considered to be DNAPLs under normal subsurface conditions may decrease during remedial actions, which impart heat to the subsurface (e.g., Johnson and Leuschner, 1992). A decrease in density of DNAPLs that have densities near that of water (e.g., some coal tar residues) may result in sufficient reduction to temporarily convert the DNAPL to an LNAPL. (Newell *et al*, 1995)

The density of water is 1000 kg/m^3 at 4°C. Most LNAPL compounds of concern at sites have densities ranging from 700 kg/m^3 to 900 kg/m^3. Most DNAPLs encountered at sites have densities ranging from 1030 kg/m^3 to 1700 kg/m^3. (AATDF, 2003)

Density is related to hydraulic conductivity by **Equation 4-1** and thus determines the flow dynamics of NAPL.

$$K = k\rho g/\mu$$ *Equation 4-1*

Where K is the hydraulic conductivity (see Section 4.4.1), k the permeability, ρ is the fluid density, g is the gravity acceleration and μ is the dynamic viscosity (see Section 4.3.2).

Density (specific gravity) determination:

Density can be determined by the methods listed in **TABLE 4-2** (Cohen and Mercer, 1993).

TABLE 4-2: Density determination

	Displacement method for solids		**Determination Densitometers**	**Density of liquids by determination**	**Specific Gravity Hydrometer**	**Certified laboratory determinations**
Requirements	Balance	Graduated cylinder	Densitometer	Balance	Hydrometer (calibrated, weighted, glass float), thermometer and cylinder	100 g solid sample, 1 L liquid sample
Costs	\$ 150 - 200	\$ 10 - 20	\$ 2000	> \$ 200	\$ 20, \$ 160 for a set of 8 with a thermometer included	\$ 10 –24 \$ 250 (includes viscosity determined at 3 temperatures)

4.3.2 Viscosity (μ))

Viscosity is the internal friction derived from molecular cohesion within a fluid that causes it to resist flow. Low viscosity NAPL will flow more rapidly in subsurface than a high viscosity NAPL, assuming all other factors is equal. The viscosity of most fluids will decrease as the temperature increases. The lower the viscosity, the less energy required for a fluid to flow in a porous medium. The hydraulic conductivity increases as the fluid viscosity decreases (Newell *et al*, 1995). Viscosity values are given in **APPENDIX A**.

Results from laboratory experiments indicated that several chlorinated hydrocarbons that have low viscosity (methylene chloride, perchloroethylene, 1,1,1-TCA, TCE) will infiltrate into soil notably faster than will water (Schwille, 1988). The relative value of NAPL viscosity and density, to water, indicates how fast it will flow in porous media (100% saturated) with respect to water. For example, several low viscosity chlorinated hydrocarbons (TCE, tetrachloroethylene, 1,1,1-TCA, Methylene Chloride, Chloroform, Carbon Tetrachloride, will flow 1.5-3.0 times as fast as water and higher viscosity compounds including light heating oil, diesel fuel, jet fuel, and crude oil (i.e. LNAPL's) will flow 2-10 times slower than water (Schwille, 1981). Both coal tar and creosote typically have a specific gravity greater than one and a viscosity greater than water (Huling and Weaver, 1991). The viscosity of NAPL may change with time (Mercer and Cohen, 1990). As fresh crude oils lose the lighter volatile components from evaporation, the oils become more viscous as the heavier components compose a larger fraction of the oily mixture resulting in an increase in viscosity (Huling and Weaver, 1991). **TABLE 4-3** shows different methods of viscosity determination.

Viscosity determination (Cohen and Mercer, 1993):

TABLE 4-3: Viscosity determintation

	Falling Ball	**Falling Needle**		**Rotating Disk Viscometer**	**Viscosity Cups**	**Certified Lab analysis**
Requirements	A set of 3 tubes – viscosity ranges: 0.2-2 cp, 2-20 cp and 20-1000 cp	Falling needle unit with glass needles, 4 inches long, measure ranges of viscosity from 10 – 24000000 cp.		Rotating disk viscometer	5 Zahn Viscosity cups, ranges: 15-78 cSt, 40-380 cSt, 90-604 cSt, 136-899 cSt, 251-1627 cSt	500 mL sample
Costs	S 120 per tube	Unit without stopwatch	Unit with stopwatch	$ 1750	$ 80 per cup	$ 30- 40 per viscosity determination (Cohen and Mercer, 1993); $ 250 (ASTM D445), three temperatures including density (PTS Geolab)
		$ 3800	$ 7900			

4.3.3 Interfacial tension (σ))

The characteristics of NAPL movement are largely derived from interfacial tension (σ), which exists at the interface between immiscible fluids. Interfacial tension is a factor directly related to capillary pressure and controls wettability (Cohen and Mercer, 1993).

Interfacial tension (and contact angle – see section 4.3.4) is needed to determine the entry pressure (Pe – **Equation 4-2**) and the minimum pool height (H – **Equation 4-3**) related with a certain fracture aperture:

$$\mathrm{Pe} = \frac{2\sigma \cos\theta}{e} \qquad \textit{Equation 4-2}$$

Where Pe is the entry pressure of interest, σ is the interfacial tension between the DNAPL and water, θ is the contact angle on the fracture walls and e is the largest fracture aperture.

$$H = \frac{2\sigma \cos\theta}{(\rho_{nw} - \rho_{w})ge} \qquad \textit{Equation 4-3}$$

Where H is the minimum pool height, σ, θ and e is the same as above, ρ_{nw} is the density of the non-wetting fluid, ρ_w is the density of the wetting fluid (water) and g is gravity acceleration.

In general, the greater the interfacial tension, the greater the stability of the interface between the liquids (Newell *et al*, 1995). The interfacial tension between a liquid and its own vapor is called surface tension. It is measured in units of energy per unit area, typically using the capillary rise or Du Nouy tensiometer methods. Oil-water interfacial tension varies as a function of the chemical composition of the oil, amount and type of surface-active agents, types and quantities of gas in solution, pH of the water, temperature, and pressure. **FIGURE 4-1** (next page) shows an interfacial tension nomograph with which one can estimate oil-water interfacial tensions at reservoir temperature (Schowalter, 1979). The lowering of interfacial tension upon increasing the temperature, may lead to easier remediation. (Keller, 1999 and EPA, 1997 (a)) TABLE 4-4 shows different methods for determining interfacial tension.

Determination of interfacial tension (Cohen and Mercer, 1993):

TABLE 4-4: Interfacial tension determintation

	Determination by capillary rise	**Du Nuoy Ring Tensiometer method**	**Laboratory testing**
Requirements	Density, other parameters measured by capillary rise measurement apparatus	Tensiometer (manual to semi-automatic units)	Not Reported
Costs	$ 65 per apparatus	$ 2200 – 2800 (Cohen and Mercer, 1993), $ 175 per phase pair (PTS Geolab)	$ 40 per sample

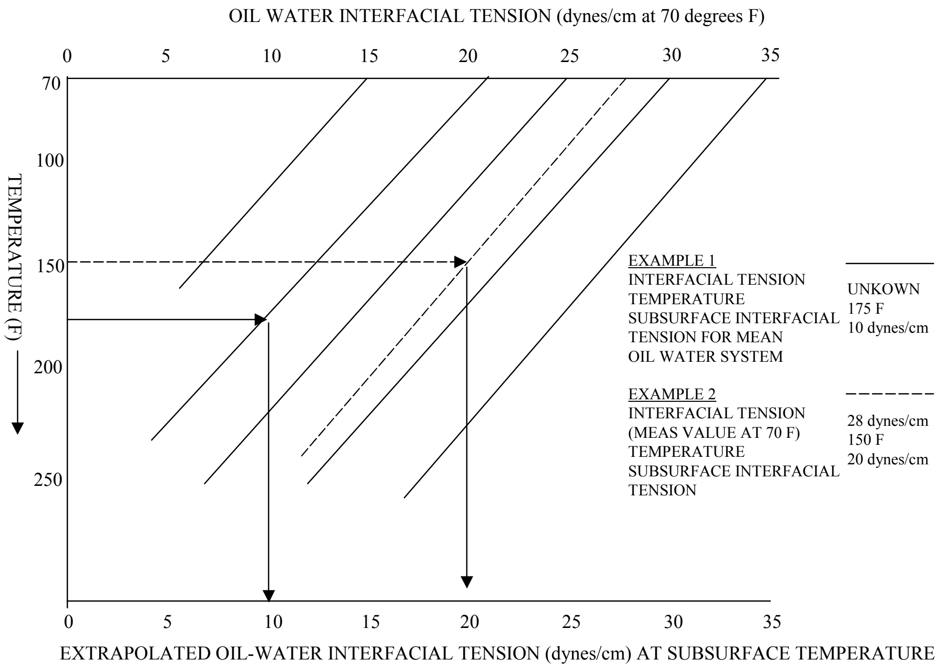


Figure 4-1 (Interfacial tension nomograph) – Schowalter (1979)

4.3.4 Wettability / contact angle (θ)

Wettability can be defined as the work necessary to separate a wetting fluid from a solid (Cohen and Mercer, 1993) or as the overall tendency of one fluid to spread on or adhere to a solid surface (i.e., preferentially coat) in the presence of another fluid with which it is immiscible (Newell *et al*, 1995).

In a multiphase system, the wetting fluid will preferentially coat (wet) the solid surfaces and tend to occupy smaller pore spaces. The non-wetting fluid will generally be restricted to the largest interconnected pore spaces. In the vadose zone, where air, water, and LNAPL are present, liquids, usually water, preferentially wet solid surfaces. However, under conditions where only LNAPL and air are present, LNAPL will preferentially coat the mineral surfaces and displace air from pore spaces. In the saturated zone, with only water and LNAPL present, water will generally be the wetting fluid and will displace LNAPL from pore spaces (Newell *et al*, 1995).

Wettability is generally expressed mathematically by the contact angle of the oil-water interface against the rock or pore wall as measured through the water phase. For rock-fluid systems with contact angles between 0 and 90°, the rocks are generally considered water-wet; for contact angles greater than 90°, the rocks are considered oil-wet. Water-wet rocks would imbibe (absorb) water preferentially to oil. Oil-wet rocks or oil-wet surfaces would imbibe oil preferentially to water. Although a contact angle of 90° has generally been considered the breakover point to an oil-wet surface, Morrow *et al* (1973) stated that a contact angle of greater than 140° in dolomite laboratory packs was necessary for oil to be imbibed (Schowalter, 1979).

Wettability determination:

TABLE 4-5: Wettability determination

	Contact angle method	Arnott method	USBM wettability index
Requirements	A needle with which to drop a small drop of NAPL on a polished surface, and a photomacrographic apparatus to take close-up photographs from which contact angles are measured	Rock core that is centrifuged in 1) water, then 2) NAPL (after which volume of H_2O displaced by NAPL is measured), then 3) core again immersed in H_2O and volume of NAPL displaced by H_2O measured after 20 hours, then 4) centrifuged in H_2O and total volume NAPL displaced, is measured.	Only applicable to porous media that can be cut into plugs for centrifugation (rock and clay). Need centrifuge.
Costs	\$ 1200 – 1500 (petroleum laboratories)	\$ 1500 (petroleum laboratories), \$ 1200 (PTS Geolab)	\$ 1500 (PTS geolab)

The approximate relationship between wettability, the contact angle and the USBM and Arnott wettability indexes is shown in **TABLE 4-6** (Cohen and Mercer, 1993).

TABLE 4-6: Relationship between wettability and contact angle

Method	Water-Wet	Neutrally Wet	NAPL-Wet
Contact angle:			
Minimum	0^0	60 to 75 ^{0}	105 to 120 ^{0}
Maximum	60 to 75 ^{0}	105 to 120 ^{0}	180^0
USBM wettability Index	W near 1	W near 0	W near -1
Arnott wettability Index			
Displacement-by-water ratio	Positive	Zero	Zero
Displacement by NAPL ratio	Zero	Zero	Positive
Arnott-Harvey wettability index	$0.3 \leq I \leq 1.0$	$-0.3 < I < 0.3$	$-0.1 \leq I \leq -0.3$

4.3.5 Solubility

Aqueous solubility reflects the maximum concentration of a chemical that is able to dissolve in pure water at a particular temperature. It is commonly reported that organic compounds are found in groundwater at concentrations less than 10 percent of the NAPL solubility limits (Cohen and Mercer, 1993), even when

NAPL pollution is known or suspected at a site, while laboratory experimental results reflect chemical concentrations approximately equal to the compound aqueous solubility (Anderson, 1988).

The reasons for these field / laboratory measurements are varied:

- When heterogeneous field conditions (non-uniform groundwater flow, stratified groundwater in boreholes) exist
- When NAPL is present is large complex ganglia, or when the groundwater flow velocity is high, that limits the dissolution rate
- When the mass fraction of soluble species in a NAPL mixture is low
- Where the NAPL is composed of multiple chemicals the mixed compound solubility is less than the pure compound solubilities.

Various factors influence the solubility of NAPL (Cohen and Mercer, 1993), which may be Temperature, Co-solvents, Salinity, Dissolved organic matter, Groundwater velocity and NAPL-water contact area.

Determination of solubility:

Solubilities may be obtained from literature, measured experimentally or estimated from empirical relationships established between solubility and chemical properties such as the octanol-water partition coefficient (Kow) and the organic carbon-water partition coefficient (Koc) (Cohen and Mercer, 1993).

For a single component NAPL, the pure-phase solubility of the organic constituent can be used to estimate the theoretical upper level concentration of organics in aquifers or for performing dissolution calculations. For mixed NAPLs, however, effective solubility should be calculated. To determine the effective solubility of a mixed compound, Raoult's Law must be used. Errors are expected for the estimation of the effective solubility when using the equation below, if a high concentration of co-solvents (such as alcohol) occurs in the mixture, which may significantly increase the solubility of the mixture (Cohen and Mercer, 1993).

$$S^e_i = XiSi \qquad \textit{Equation 4-4}$$

Where

S^e_i = Effective solubility (the theoretical upper-level dissolved-phase concentration of a constituent in groundwater in equilibrium with a mixed NAPL, in mg/l)

Xi = the mole fraction of component I in the NAPL mixture (obtained from lab analysis of a NAPL sample or estimated from waste characterization data)

Si = the pure-phase solubility of compound i in mg/l (literature).

This relationship is approximate (ideal) and does not account for non-ideal behaviour of mixtures, such as co-solvency.

Determination of the **Mole Fraction**

$x_o = MF_x \, MW_o \, / \, MW_x$ *Equation 4-5*

MF_x = mass fraction of selected chemical in mixture
MW_o = average molecular weight of mixture
MW_X = molecular weight of selected chemical (EPA (d), 2003)

In order to determine the mass fraction of a selected chemical in a mixture, the total mixture must be analysed and the different fractions of mass of each chemical determined. The determination of the molecular weight of a mixture is also problematic for many laboratories. Usually an on-site industrial process laboratory can determine these variables, where normal labs are not equipped to determine these variables. In South Africa no known laboratory can analyze for these constituents.

At sites with complex or varied NAPL mixtures, or where samples can not be obtained from analysis, a reliable estimation of effective solubilities will be confounded by deficient knowledge of the NAPL composition (mole fractions). In this case, bounding assumptions have to be made regarding the composition in order to determine the range of possible effective solubilities.

4.3.6 Saturation and residual saturation

The saturation of a fluid is the volume fraction of the total void volume occupied by that fluid. Saturations range from zero to one and the saturations of all fluids sum to one. Saturation is important because it is used to define the volumetric distribution of NAPL. Other properties like relative permeability and capillary pressure are also functions of saturation (Cohen and Mercer, 1993). The mobility of an LNAPL is related to its saturation in the medium as described by the relative permeability function.

Residual Saturation

Residual saturation is defined as the volume of hydrocarbon trapped in the pores relative to the total volume of pores and therefore is measured as such (Huling and Weaver, 1991). Residual saturation has also been described as the saturation at which NAPL becomes discontinuous and is immobilized by capillary forces (Huling and Weaver, 1991).

Residual saturation of for instance an LNAPL represents a potential source for continued groundwater contamination that is tightly held in the pore spaces and not readily removed using currently available remediation technologies. The magnitude of residual saturation is affected by several factors including pore-size distribution, wetting properties of the fluids and soil solids, interfacial tension, hydraulic gradients, ratios of fluid viscosities and densities, gravity, buoyancy forces, and flow rates (Mercer and Cohen, 1990; Demond and Roberts, 1987 and 1991). Some researchers reported that residual saturation values appear to be relatively insensitive to fluid properties and very sensitive to soil properties (and heterogeneities) (EPA, 1990). Results of laboratory experimentation indicated that residual saturation increased with decreasing hydraulic conductivity in both the saturated and unsaturated zones. Due to the known heterogeneity of subsurface systems with regard to these factors, it follows that residual saturation in the subsurface is also highly variable. Data compiled by Mercer and Cohen (1990) indicate the residual saturation of most NAPLs in these studies ranged from about 10% to 20% in the unsaturated zone and about 15% to 50% of the total pore volume in the saturated zone.

Saturation determination:

NAPL saturation can be determined in the following ways:

Extract NAPL from soil by shaking a soil and water suspension sample together with a strip of hydrophobic porous polyethylene in glass jar for several hours (Cary et al, 1991). The method relies on water to displace organic compounds from hydrophilic soils and porous polyethylene to absorb the displaced organic liquid. The method is reported to be applicable in the field and VOCs, SVOCs and non-volatile organic compound should be determined by the method. A short description is given:

- Cut several strips of porous polyethylene having a pore size of 10 to 20 μm. At least 1 g dry polyethylene is needed per 0.5 ml of NAPL in the sample.
- Oven-dry the strips, record their weights and pre-treat the strips by wrapping in oil-wet tissue paper. The oil treatment ensures maximum hydrophobicity.
- Weigh 20g of the soil sample and place it and a polyethylene strip in a 50 ml glass vial fitted with a Teflon cap.
- Add 20 ml of water in the vial and stopper the vial. Rock on a mechanical shaker for 3 - 4 hours.
- Remove the strip from the vial, wash particles from strip with water and brush off water droplets with tissue paper. Weigh strip and determine mass absorbed.
- Oven dry soil for 12 hours (105°C) to determine initial water content of sample.
- Determine percent saturation of water and NAPL.

Saturation can also be determined gravimetrically by solvent extraction and distillation processes (Amyx *et al*, 1960). The most general method is to extract organics with organic solvent (methanol / ethanol) and to do a gravimetric (HPLC) determination of saturation. For this analysis laboratories need 1 kg solid sample (Cohen and Mercer, 1993).

The Modified ASTM method (using the Dean-Stark apparatus) is a petroleum industry method. This process is essentially a distillation. The core can be completely cleaned to produce a clean dry sample for porosity and other tests (Amyx *et al,* 1960).

Water saturation can be determined directly by measuring the volume of condensed water and dividing by the sample porosity. NAPL saturation is determined indirectly by weighing the core sample prior to extraction and then again after extraction, cleaning and drying of the core sample, by the following equation:

$$Sn = (M_T - Md - Mw) / (V_n/\rho_n) \qquad \textit{Equation 4-6}$$

Mt = wet sample mass
Md = dry sample mass
Mw = extracted water mass
V_n = sample pore volume
ρ_n = NAPL density

The costs of different analysis per sample are shown in **TABLE 4-7** (Cohen and Mercer, 1993):

TABLE 4-7: Saturation determination

	Gravimetric analysis	Chemical analysis (sample without chlorinated solvents)	Chemical (sample containing chlorinated solvents)
Cost	$ 300 - 800	$ 25	$ 500

4.4 NON-NAPL PHYSICAL PARAMETERS AND DETERMINATION

4.4.1 Hydraulic conductivity (K)

This parameter is a measure of an aquifer's ability to transmit water and is one of the most important variables governing groundwater flow in aquifers. Hydraulic conductivity has the units of length over time (L/T) and is highly variable. Reported values of K range over 10 orders of magnitude, from 3×10^{-9} to 3×10^{2} m/day (Domenico and Schwartz, 1998 - Table 1). In general, K values for unconsolidated sediments tend to increase with increasing grain size. The velocity of groundwater and dissolved contaminants is directly related to K. Variations in K directly influence the fate and transport of the contaminant by providing preferential migration pathways (Nanh *et al,* 2000). See **TABLE 4-8** for typical hydraulic conductivity values.

TABLE 4-8: Typical hydraulic conductivity values	
Materials	**Hydraulic conductivity (m/day)**
Glacial Till	9×10^{-8} to 2×10^{-1}
Clay	9×10^{-7} to 4×10^{-4}
Silt	9×10^{-5} to 2
Fine sand	2×10^{-2} to 20
Medium sand	8×10^{-2} to 50
Coarse sand	8×10^{-2} to 500
Gravel	30 to 3000
Karstic limestone	9×10^{-2} to 2000
Limestone and dolomite	9×10^{-5} to 0.5
Sandstone	3×10^{-3} to 0.5
Siltstone	9×10^{-7} to 1×10^{-3}
Shale	10^{-9} to 2×10^{-4}

Domenico and Schwartz, 1990

4.4.2 Retardation factor (R)

Kd is used in the determination of movement of dissolved plume phase, for instance in the determination of the Retardation factor:

$R = [1 + (\rho_b/n)Kd]$ *Equation 4-7*

Where ρ_b is the bulk density (Section 4.4.3), n is the porosity (Section 4.4.4) and Kd is the distribution coefficient (Section 4.4.2.3)

4.4.2.1 Organic carbon partition coefficient (Koc)

Koc (organic carbon partition coefficient) is an indicator of a chemical's tendency to partition between groundwater and soil and is expressed in (mL/g). This value can also be seen as a soil adsorption coefficient. A low Koc will indicate low soil adsorption, thus contaminants with a low Koc will leach faster from a landfill site than high Koc contaminants.

Koc < 50	Slight adsorption and high leaching capacity
Koc 50-200	Moderate adsorption and leaching capacity
Koc > 200	Strong adsorption and slight leaching capacity (DWAF (b), 1998)

Textbook values exist for certain organic chemicals, but where not available, Koc can be estimated from the log Kow (Octanol water partition coefficient, which is related to hydrophobicity):

$\log Koc = a \log Kow + b$ (Pankow and Cherry, 1996) *Equation 4-8*

A compound with a high Kow is considered relatively hydrophobic and would tend to have low water solubility, a large soil/sediment adsorption coefficient, a large retardation factor and a large bio-concentration factor (University of Texas, 2004). Parameters a and b as well as c and d (Eq. 4-9) are empirical, compound class parameters derived by regression of available data (Pankow & Cherry, 1996) .

Koc can also be estimated from solubility:

$\log Koc = c \log S + d$ (Pankow and Cherry, 1996) *Equation 4-9*

Parameters a, b, c and d are empirical parameters derived by regression of available data (Pankow and Cherry, 1996). Some of the most commonly used regression coefficients from literature were obtained by Karickhoff (1981, 1984). The above equations apply the best for sorption to soils in cases where the foc is larger than 0.001 (Schwarzenbach and Westall, 1981).

Values for coefficients a, b, c and d is given in **TABLE 4-9.**

TABLE 4-9: Koc determination – values for coefficients a, b, c and d

Compound class	**a**	**b**	**c**	**d**	**Reference**
Nonaromatic, halogenated compounds	0.827	-0.039	-0.346	1.28	Gerstl (1990)
Aromatic, halogentaed compounds	0.722	0.417	-0.475	0.839	Gerstl (1990)
TCE, PCE, DCB and benzene on low foc solids	0.69	0.22			Piwoni and Banerjee (1989)

The Koc is used to determine Kd as shown in equation 4-9:

$Kd = koc \times foc$ (Pankow and Cherry, 1996) *Equation 4-10*

Foc and it’s determination is discussed in Section 4.4.2.2.

The Kd value can be used to determine the retardation factor (Section 4.4.2 – *Equation 4-7*). An example can be seen in section 4.1.

4.4.2.2 Fraction of organic carbon (Foc)

Fraction of total organic carbon content is expressed in terms of grams of organic carbon per gram of soil (g/g), and is expressed as a decimal. TOC is expressed as a percentage (Vance, 2003). In natural soil foc values range from <0.001 to >0.05 (Cohen and Mercer, 1993). The Agricultural Research Council (ARC) can determine TOC, from which foc can be determined. See **TABLE 4-11**, section 4.5, for prices and requirements for analysis. Textbook Foc values are listed in **TABLE 4-10**.

TABLE 4-10: Typical foc values

Material	foc	Reference
Medium sand	0.00017	Spitz, Moreno (1996)
Fine to med sand	0.00023	Spitz, Moreno (1996)
Fine sand	0.00026	Spitz, Moreno (1996)
Silt	0.00108	Spitz, Moreno (1996)
Sand, gravel	0.0004 to 0.0073	Spitz, Moreno (1996)
Sediment eutrophic lake	0.019 to 0.058	Spitz, Moreno (1996)
Coarse soil	0.042	Vance (2003)
Clayey silt loam	0.004	Vance (2003)
Silty Loam	0.016	Vance (2003)
Silty Clayey Loam	0.0295	Vance (2003)
Silty Loam	0.052	Vance (2003)
Clayey Loam	0.0038	Vance (2003)
Glaciofluvial	0.0002 to 0.01	Vance (2003)

4.4.2.3 Distribution coefficient (Kd)

The equilibrium distribution coefficient (Kd) is commonly predicted (for non-ionic organic compounds) by equation 4-10.

$Kd = koc \times foc$ *Equation 4-11*

The determination of Koc and foc values are described in Sections 4.4.2.1 and 4.4.2.2.

4.4.3 Bulk density (p_b)

Bulk density is a measure of the weight of the soil per unit volume (g/cc), usually given on an oven-dry (110° C) basis. Most mineral soils have bulk densities between 1.0 and 2.0. Bulk density can be determined from porosity in the following way:

$\text{Porosity } \% = 1 - (\text{Bulk density} / \text{particle density}) \times 100$ (IUPUI, 2004) *Equation 4-12*

Thus

$\rho b = \rho s\,(1\text{-}n)$ *Equation 4-13*

Where n = porosity, ρ_b = bulk density, p_s = particle density (on average 2.65 g/cm^3 for most mineral soils – IUPUI, 2004; Cohen and Mercer, 1993)

4.4.4 Porosity (n)

Percent porosity = 100 x (bulk volume - grain volume/bulk volume) OR Percent porosity = 100 x (pore volume/bulk volume) Several methods exist for porosity determination, e.g. bulk volume determination and the pore gas expansion method. Bulk volume determination: The bulk volume of the extracted and dried samples may be determined by volumetric displacement of mercury. Pore gas expansion method: The measurements of porosity may also be made by the pore-gas expansion method, or the so-called Washburn-Bunting method (1922). This method makes use of a modified Toepler pump so much in use in high-vacuum techniques in order to produce the barometric vacuum and remove air from a dried core. The bulk volume of the core must be known from other tests (Physics - Instant Essays, 2004).

4.5 SOUTH AFRICAN LABORATORIES ANALYSES CAPABILITIES

Queries have been directed to the institutes with analysis laboratories, which are listed in TABLE 4-11:

TABLE 4-11: South African laboratories analyses capabilities

Laboratory	**CSIR**[1]	**ARC**[2]		**Khanya**[3]	
		Cost	**Sample Size**	**Cost**	**Sample Size**
Saturation	No	No	N/S	No	
Density	No	No	N/S	R 25 (R100 admin, handling reporting fee)	250 ml
Viscosity	No	No	N/S	No	
Interfacial tension	No	No	N/S	No	
Mole fraction of a component in a NAPL mixture	No	No	N/S	No	
Wettability	No	No	N/S	No	
Bulk density (disturbed sample)	No	R 18	N/S	No	
Cation exchange capacity	No	R130	N/S	No	
Soil texture (7 fractions)	No	R95	N/S	No	
Drying sample	No	R 16	20 g	No	
Crushing, grind sample	No	R 8 – R 12		No	
Foc	No	R 50		No	

1. CSIR, 2003; 2. ARC, 2003; 3. Khanya, 2003 N/S = Not Specified

4.6 RESULTS AND CONCLUSIONS

The following conclusions can be drawn

- NAPL parameters (e.g. Koc, Kow) have been given in APPENDIX A. It could be seen that the availability of these parameters is sometimes questionable, and where different sets of parameters exist due to laboratory testing, there may also be huge differences in the value ranges. This has a large implication on the use of these parameters in models, and the parameters should be used with care.
- The physical differences between DNAPL and LNAPL have a significant influence on the contaminant spread and remediation possibilities of these two types of contaminants (section 4.2).
- The different properties that were listed in sections 4.3 and 4.4 find application in the determination of the movement, degradation and reactions of organic pollutants in the aquifer. Application of these parameters can be seen in chapters 6, 7 and 8.
- Laboratories in South Africa are not equipped to perform all the analyses required to sufficiently characterize NAPLs and the physical properties of the soil / rock which the NAPL is associated with. Currently, samples have to be sent overseas for analysis, which is costly and time-consuming.
- Analysis apparatus at laboratories will have to be upgraded to a certain standard and laboratories will have to be certified and accredited. This can be achieved by writing certain policies or regulations specifying certain laboratory standards. The government can set up one such laboratory with the required analysis apparatus and knowledge, and encourage laboratories to upgrade by giving certain incentives such as subsidies for certain costly apparatus or tax deduction if laboratories bought certain costly analysis apparatus. A local lab, if first set up locally, would imply cost-savings and would save large amounts of time on sending samples abroad.

Chapter 5

NAPL Site Assessment

5.1 INTRODUCTION

The determination of NAPL physical parameters and site parameters (discussed in Chapter 4) find application in site assessment and site characterization. At a first glance, site assessment and site characterization appear to be synonymous. In this chapter it will be aimed to outline the difference between the two and to stress the importance of NAPL site assessment before site characterization is performed. Chapter 6 will outline site characterization tools and their distinct uses.

The main motivation for performing a Site Assessment is that the NAPL investigations are very costly. A Site Assessment can be seen as a generic first phase, as supported in literature (EPA, 2005; Utah State University, 2005). The site assessment will give guidance for detail investigations needed on the site characteristics. With regard to the South African hard rock environment it is of paramount importance to form a conceptual model, which is refined during the Site Characterization Phase. It goes without saying that this will prevent significant financial losses.

The United States Environmental Protection Agency (USEPA) has a three-tiered Environmental Site Assessment (ESA) process and calls Site Assessment a Phase I Site Assessment, and Site Characterization a Phase II Site Assessment. The steps included under these phases are as follows:

Phase I Environmental Site Assessment:

Phase I involves a preliminary environmental review including: (1) an evaluation of the site history; (2) an assessment of pertinent regulatory compliance issues; and (3) a field reconnaissance inspection. From this work, tentative conclusions or recommendations are developed. Based on the Phase I findings, usually presented in report format, the site assessment will either be terminated or continued on to a more detailed level of investigation (Envirotools, 2004).

Phase II Environmental Site Assessment:

The next level of an ESA is Phase II. This is the start of the field investigation that is needed in order to determine if the known or suspected impacts to the environment are above regulatory levels and will need corrective action. Phase II utilizes information compiled in Phase I to develop a detailed, site-specific sampling and analysis strategy that will target suspected or known site contamination. The goal of the sampling strategy is to identify particular hazardous or non-hazardous constituents that may be present at the site, to evaluate the extent of contamination and its risk implementation, if any, and to estimate the financial impact to parties pursuing the transaction.

The three-phase ESA process (where the phases are as follows: Tier 1 = transaction screening, Tier 2 = Phase I ESA and Tier 3 = Phase II ESA) is sometimes thought to be a discrete set of steps that takes place in all cases. However, the process discussed is just that, a process. Depending on the particular set of conditions, the user must determine what components of the ESA process should be completed. For instance, if a previous Phase I was completed and it was determined that known contamination exists on-site, the project may begin with Phase II sampling. However, for a new site where nothing is known, the general three-tiered process is usually followed (Envirotools, 2004).

Rapid site assessment tools also exist by which some of the phases of site assessment and characterization can be excluded to save costs which can be implemented during site remediation. A study has been conducted to determine what amount of cost savings can be incurred by using rapid site assessment tools (Applegate and Fitton,1997). The study found the following:

Using rapid assessment tools, geological and geohydrological evaluation, on-site soil and groundwater and chemical analyses, and experienced in-field decision-making, rapid site assessment can be completed in a fraction of the time needed for full site assessment and characterization. The cost savings is incurred by using mobile laboratories, direct push technology etc., which are more costly than conventional technologies, but save numerous mobilizations, which require several cost estimates and work-plans. Savings is also made in terms of less time spent (which may imply 30-50% cost-savings) (Applegate and Fitton, 1997). Known mobile laboratories that can be hired do not exist locally and the closest representative that could be found was the Department of Water Affairs' laboratory truck, owned by the Directorate: Hydrological Services (Sub-Directorate: Groundwater Resource Assessment and Monitoring (GRAM)). It could be feasible for laboratories to set up mobile units.

5.2 PHASES OF SITE ASSESSMENT

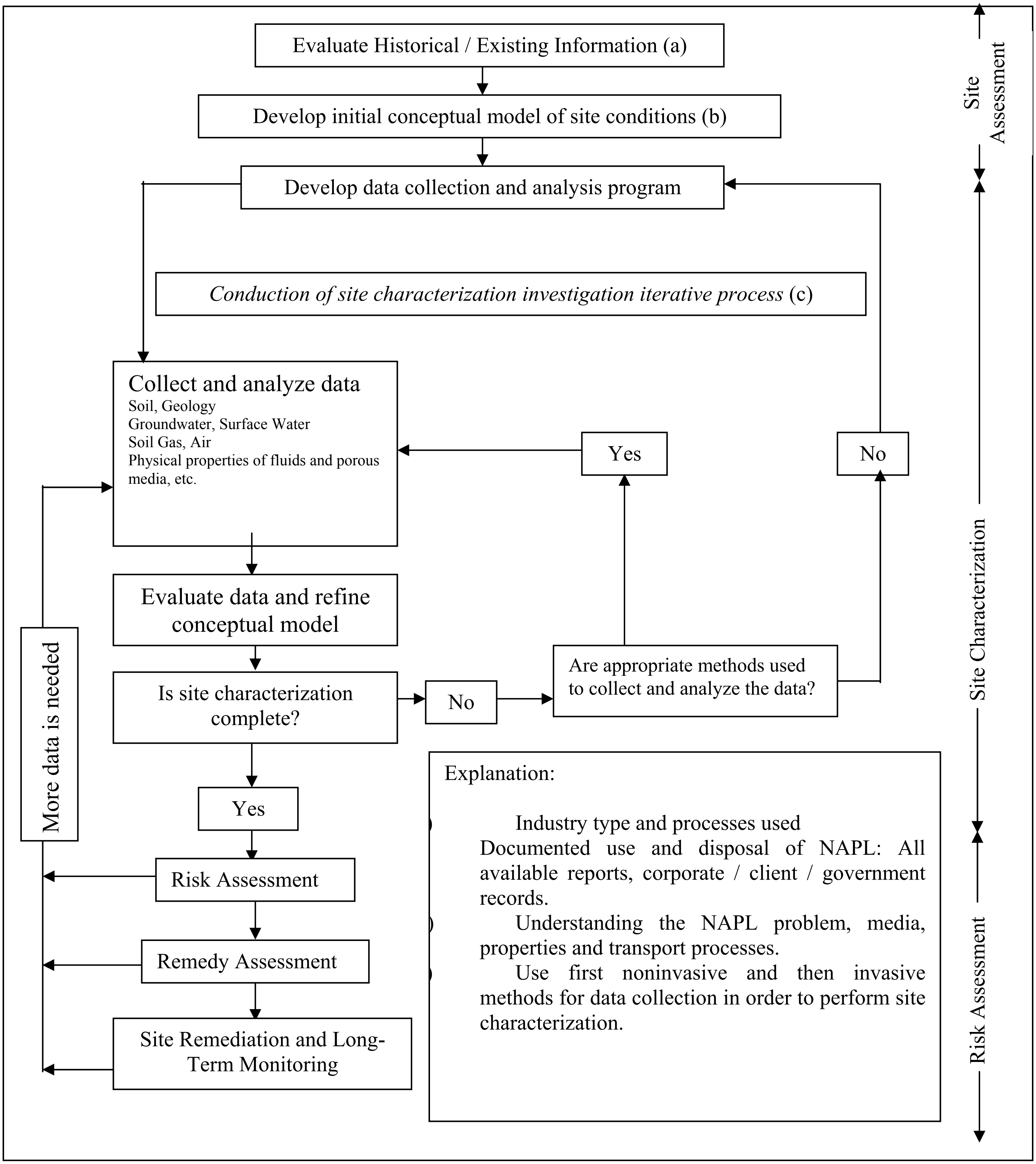
The phases of site assessment as it may be applied in South Africa, may vary according to each site, but the following steps below, may serve as a guideline in the way in which site assessment can be conducted:

- Desktop study
- Site inspection
- Inspection of surrounding environment (including hydro-census)
- Geophysical exploration
- Chemical analyses of groundwater
- Drilling of initial pilot boreholes (optional for site assessment and can form part of site characterization only, if existing data is enough for forming the initial conceptual model)
- Forming the conceptual model
- Compilation of the site assessment report
- Report submission to authorities (if required)

- Emergency system design and commissioning
- Site assessment report evaluation

Figure 5-1 (a generic flow-chart) outlines the site assessment and site characterization phases.

Figure 5-1 (Site assessment and site characterization - steps to be followed)



Explanation:

Industry type and processes used

Documented use and disposal of NAPL: All available reports, corporate / client / government records.

Understanding the NAPL problem, media, properties and transport processes.

Use first noninvasive and then invasive methods for data collection in order to perform site characterization.

The steps to be followed when performing site characterization will depend on the site assessment that has already been performed. Site-specific factors such as history, geology and type of pollutant will play a role. The iterative process shown in Figure 5-1 is applicable for instance for the drilling of boreholes to obtain different levels of information.

5.2.1 Desktop study

The purposes of desktop reviews are to:

- identify potential subsurface contaminants and environmental concerns at the site;
- identify subsurface conditions (by reviewing existing and historical data) and develop a conceptual model of the site, e.g. groundwater flow direction, subsurface geology and hydrogeology; and
- establish the framework for the subsequent site investigation and work plan (Saskatchewan Petroleum Industry,1999).

The desktop study will include much historical data, of which the following can be obtained:

Aerial photographs:

Historical and current aerial photographs must be used to determine the land-use pattern change for the operational time of the industry. Waste dumps are likely to have moved, new buildings will have been built and the processes will also have changed. The newest aerial photographs will also have to be studied to determine how much the industry has spread laterally. If the NAPL is mobile, vegetation patterns to visually detect pollution spread, can be studied.

Data from the industry:

Data such as volumes released, release times and processes must be obtained from the industry. If up to record data does not exist, this has to be estimated. If possible, the chemical make-up of the waste can also be obtained from the industry (process engineers) - in the case where industries produced chemical waste by-products, mostly in the form of DNAPL. In the case of leaking service stations, the chemical make-up will be that of the products sold at the service station (petrol and diesel, mostly LNAPL.

Regulatory information:

Information like past land-uses can be determined from authorization records at the authorities like DWAF, DME and DEAT. Existing permits / licenses can also be obtained from these authorities. Some industries, however, may still be non-compliant in terms of current legislation, and their water uses have not been registered, permitted or licensed, in which case this information will not be available at the authorities.

In **TABLE 5-1** a recommended record review is given.

<table>
<tr><th colspan="4">TABLE 5-1: Recommended record review</th></tr>
<tr><td colspan="2">RECORD TO BE REVIEWED</td><td>INFORMATION SOUGHT</td><td>SOURCE OF INFORMATION</td></tr>
<tr><td colspan="2">Aerial photographs</td><td>general site plan, and site usage, changes in land-use</td><td>Archives and company records</td></tr>
<tr><td rowspan="2">Data from industry</td><td>Company records</td><td>site plans, spill reports, audits, monitoring data</td><td>Company record files</td></tr>
<tr><td>Geological and geohydrological reports</td><td>groundwater flow and depth, subsoil type, conduits (fractures), topography</td><td>Company record files</td></tr>
<tr><td colspan="2">Regulatory information</td><td>Existing permits / licenses, exemptions</td><td>Regulators / company</td></tr>
</table>

5.2.2 Site Inspection

The purpose of the site inspection is to:

- identify visual signs of on-site and off-site soil contamination (e.g., surface staining, reduced vegetative growth and visible salt crystals);
- identify equipment and infrastructure to be decommissioned and potential sources of contamination;
- identify surrounding land use, topography and vegetation; and
- identify nearby surface water and water wells.
- identify and mark underground utilities that may be affected prior to subsurface investigations.

This information can be used to confirm site remediation requirements, to assess the environmental sensitivity of the site with respect to the potential receptors or future land use and to identify sources and potential locations of the contamination (Saskatchewan Petroleum Industry, 1999).

5.2.3 Inspection of surrounding environment (including hydro-census)

Perform a survey of surrounding sources, pathways and receptors for a 1km, 2km and 3km radius subject to catchment boundaries.

This is necessary in order to determine who the neighbouring industries are, what contributions they make towards contamination, what ground and surface water users exist in the area and what the state of the ecosystem is (DWAF, 2003).

5.2.4 Geophysical exploration

The contaminant plume (dissolved phase) can sometimes be outlined by certain geophysical techniques. This may result in significant financial savings in terms of the amount of boreholes that need be drilled. The principal geological structures can also be identified by geophysics. This is called non-invasive geophysics and is used during the site assessment phase. The different non-invasive geophysical techniques, its advantages and disadvantages and applicability in different environments, can be seen in **TABLE 5-2**. Invasive geophysics (geophysical borehole logging) is used during the site characterization phase (see Chapter 6, section 6.5).

TABLE 5-2: Different non-invasive geophysical methods, applicability for NAPL and hard rock and advantages and disadvantages								
Method		**Fractured Rock**	**Unconsolidated formation**	**DNAPL**	**LNAPL**	**Advantages**	**Disadvantages**	**References**
Surface geophysics to delineate NAPL	Electrical Impedance Tomography (EIT)	Unknown	Limited	✓ Being tested for DNAPL	✓	Effective at depths of 3-150 m Uses 50-75% less boreholes than conventional sampling technologies Effective at mapping leaks from underground tanks, plumes of contamination	Implementation costs range widely Possible adverse effects by steel centralizers in monitoring wells and/or steel well casings. PVC cased well or open borehole is recommended. Possible adverse effects related to pipelines and/or buried power lines located close to borehole. Not as effective in consolidated and unconsolidated rock. Better results in sands, silts, clay tills, etc. Unable to differentiate between type of contaminant.	ITRC, 2000
	High resolution 3D electromagnetic (EM) resistivity survey	✓	✓	Inconclusive	✓	Non-invasive technology Reduces time & expenses Serve to identify high resistivity anomalies which are representative of locations that may contain DNAPL. Can be used to monitor mediation operations efore and after surveys).	Requires thorough understanding of local geology Not a standalone method, need chemical confirmation samples Grid edge effect present difficulties in field applications EM survey area limited to 100 ft (90m) radius around each hole, thus need suspected NAPL location to be effective Depth of well limits the investigation depth May only identify 60 to 80 percent of the NAPL plume due to complex subsurface lithology.	ITRC, 2000, CIRIA, 2000
	High resolution 3D Seismic reflection survey	✓ Especially structures	✓	None (normal seismic reflection)	None	Full imaging of LNAPL sites by generating 3D high resolution images Detect fractures and channels that serve as preferred pathways for DNAPL migration after a spill.	The technology does not specifically detect DNAPLs; merely detects fractures and channels that may serve as preferred pathways for DNAPL migration. Spatial resolution may preclude use to delineate DNAPL in ganglia configurations. Not a stand-alone process, so it must be calibrated to hard data.	ITRC, 2000

TABLE 5-2: Different non-invasive geophysical methods, applicability for NAPL and hard rock and advantages and disadvantages *(contd.)*

Method		Fractured Rock	Unconsolidated formation	DNAPL	LNAPL	Advantages	Disadvantages	References
Geophysics to delineate subsurface	Ground Penetrating Radar (GPR)	✓	✓	Limited	Limited	Good for non-metallic wastes delineation Depth and thickness of soil and rock layers delineation Can identify underground storage tanks	Less than 30 ft depth penetration (100 ft under ideal conditions) Penetration limited by increasing clay content and fluid conductivity Inability to produce direct readings or measurements. NAPL concentration must be fairly high, so may be limited to identifying plume source	Cohen and Mercer, 1993 ITRC, 2000
	Electromeganetic Conductivity (EM)	✓ Especially structures	✓	Limited	Limited	Good for non-metallic wastes delineation Very rapid profiling and mapping	Affected by cultural features (metal fences, buildings, vehicles)	Cohen and Mercer, 1993
	Electrical Resitivity	Limited	✓	Limited	Limited	Delineate metallic waste, depth to landfill base Soundings and profiling	Requires good ground contact & long electrode arrays Integrates large volumes of subsurface Affected by cultural features	Cohen and Mercer, 1993
	Magnetics	✓ Especially structures	✓ If structures run through unconsolidated media	Limited	Limited	Good for metallic wastes delineation, magnetic structures and depth to base of landfill	Only applicable in certain rock environments Limited by cultural metal features	Cohen and Mercer, 1993
Soil gas analyses		Limited	✓	Limited, only vadose zone and interface zone areas	✓	Indirect evidence based on VOC detection in vadose zone Very high concentrations (approaching saturated vapor concentrations) may be indicative of DNAPLs present in vadose zone adjacent to the sampling point	Subaqueous DNAPL may not easily volatilize Not generally depth specific due to migration characteristics of materials Preferential pathways can lead to misinterpretation Poor correlations between soil gas concentration and soil concentrations False negatives possible since vapor concentrations can rapidly decline due to transport by diffusion	Rivett, 1995 Rivett and Cherry, 1991 EPA, 1987 Marrin 1988; Marrin and Kerfoot 1988; Cohen and Mercer, 1993 Devitt *et al*, 1987 Downey and Hall, 1994

5.2.5 Chemical analyses of groundwater

Analyses of macro and micro-elements can be conducted on existing boreholes (DWAF, 2003). The selection of variables to be analyzed will be site-specific, but will include analyses of inorganic and organic variables. This information will be used to form the initial conceptual model. If no boreholes exist, boreholes will have to be drilled.

5.2.6 Drilling of initial boreholes

If no boreholes exist at all, a few must be drilled to aid in the formation of the conceptual model. In the site characterization phase, the model can then be refined (or changed) and more (site-specific) data generated. The initial boreholes drilled in the site assessment phase, will inevitably be used in the site characterization phase as well.

5.2.7 Forming the conceptual model

The conceptual model can be formed once the basic data required, has been collected (DWAF, 2003). This conceptual model will inevitably be very crude and it is not recommended that site-specific predictions be made from this model. It can aid the industry and the authorities, however, in setting the constitutional controls in place.

5.2.8 Compile site assessment report

The compiled site assessment report may include the following topics. However, some of these topics will only be addressed after site characterization has been performed and the final conceptual model has been drawn up.

- Initial conceptual groundwater model
- Groundwater aspect and impact register
- Source description
- Pathway description
- Receptor description
- Possible impacts
- Possible remedies
- Monitoring requirements (the site assessment phase will identify initial monitoring requirements but the initial monitoring plan will not be the final monitoring requirements for site closure and remediation).
- Requirements of base line study (covered during the site characterization process) and the proposed study plan
- Requirements for the process to be followed – subject to regulatory authorities
- Time frames for the study phases to follow

- Requirements for emergency actions (if needed, and these will be risk based (DWAF, 2003))

5.2.9 Report submission to authorities

The site assessment report is submitted to the authorities for discussion and agreement on ways forward and time frame for execution (DWAF, 2003).

The DWAF can specify certain technical requirements for site characterization and remediation. These requirements could be:

- How site characterization should be preformed (e.g. following an outside-in approach for drilling in NAPL areas)
- The type of chemical laboratory analyses required (e.g. using a certified ISO 14000 laboratory, and specifying what the detection limits should be)
- To what degree the site should be remediated (e.g. specifying resource quality objectives (RCO's) for water released into water courses from the NAPL site) – this is only applicable after it has been decided if and what type of remediation is going to be performed (i.e. after having performed site assessment and characterization).

5.2.10 Emergency system design and commissioning

The emergency measures (if required) are designed and commissioned after discussion and agreement with the authorities (DWAF, 2003). This phase must be initiated before site characterization commences in order to address any contamination sources that may already be removed / contained.

5.2.11 Site assessment report evaluation

Upon completion of the site assessment report, an evaluation of the information should be carried out to answer the following questions:

- Is sufficient information available to conclude the likelihood that the contamination (on-site and in the surrounding area) is a result of the operations carried out on the site (or do other sources exist)?
- If contamination is present, is there sufficient information available to comment on the extent of contamination?
- If further investigation (site characterization) is not intended, is there sufficient information to satisfy the receptors (land-owners and stakeholders, the environment) and the government? (Saskatchewan Petroleum Industry, 1999)

5.2 CONCLUSIONS

Site assessment is a necessary first step of site characterization, where the site characterization should be seen as a refinement of the conceptual model. Site assessment should be conducted at every site before site characterization since this could lead to large cost savings.

The site assessment of each site will be specific and will depend on the characteristics of the site. As such, there is no fixed recipe to follow for performing a site assessment. A must for each site, is the site visit. By only conducting a desktop study from the office one could miss pollution sources not mentioned in previous industry reports.

Most sites will require sampling and chemical analyses, but for some sites a few initial boreholes will need to be drilled where at other sites existing boreholes that meet the sampling requirements can be used. The drilling of a few initial boreholes should not be seen as an unnecessary expenditure during site assessment since these boreholes give invaluable information needed for the site conceptual model, and on making decisions regarding extra boreholes, their placement and drilling them in such a manner as to prevent NAPL contamination spread.

The use of geophysics (if the site allows it) is recommended since this could lead to cost-savings when drilling boreholes. If geophysics is going to be performed outside the site, the extrapolation of data across the site should be approached with care. Geological variation could occur over small areas and the extrapolation and subsequent interpretation of site conditions using geophysics could be wrong. It should be remembered that geophysics is still just an interpretation tool for subsurface conditions and boreholes should be drilled where the site allows it, to confirm the interpretation of geophysical results.

Many new technologies exist by which NAPL pollution can be delineated in the subsurface (see Chapter 6, Section 6.5). Some of these technologies, however, are in their development phase and results are not guaranteed. As such these technologies may incur larger costs for industries in developing countries like South Africa and should be applied with care. Depending on the site, it may be more cost-effective to drill a few more boreholes than to apply such a technology.

The use of rapid site assessment technologies may not be feasible in South Africa since these technologies are not readily available (to buy or to hire), which may lead to more expenditure rather than cost savings.

Chapter 6

Site Characterization

6.1. INTRODUCTION

Building on Site Assessment, site characterization is a much more detailed investigation. Where certain studies have already been performed in the site assessment phase and an initial conceptual model has been drawn up, large costs savings may be implied. Crucial data gaps will be filled during the site characterization phase and the initial conceptual model drawn up during site assessment will be refined and tested. The nature of the site characterization study will be determined by:

1. Money,
2. Legal Framework,
3. Specific negotiations with authorities, and
4. Specific Site Characteristics (e.g. geology, land-use)

Considering financial and legal aspects, the methods of characterization will determine the reliability of the information generated. Data reliability is crucial for the risk assessment and remediation phases.

This chapter focuses on methodologies for Site Characterization. Difficulties encountered during site characterization will be highlighted. The different site characterization methods (including geophysical techniques, visual tests, drilling, and chemical analyses to be performed) will be listed in **TABLE 6-2**. The applicability in the fractured rock environment will also be highlighted since South Africa is largely a hard rock environment. Well, soil and pollutant tests that can be considered during site characterization are also listed in **TABLES 6-3** to **6-5**. In Chapter 7 an example of site characterization under typical South African circumstances with industries that one might typically encounter is given.

6.2 OBJECTIVES / STRATEGIES OF SITE CHARACTERIZATION

The definition of site characterization: Site characterization is performed in phases and is a process in which scientific method is followed. During the initial phase a conceptual model of the chemical presence, transport and fate is formulated based on available site information and an understanding of the processes that control chemical distribution (called site assessment), and described in Chapter 5 (Cohen and Mercer, 1993). Data collection commences as the second phase (site characterization) to test and improve the site conceptual model and facilitate risk assessment. As such, the site characterization efforts should focus on obtaining data needed to implement potentially feasible remedies. After data have been obtained and analyzed, the hypothesis is improved by means of iteration (Cohen and Mercer, 1993). In **TABLE 6-1** the objectives of NAPL site characterization is described.

Objectives of NAPL site characterization:

To determine NAPL properties and composition, in order to delineate the solute, mobile and residual DNAPL, as well as the mobility of the DNAPL (Cohen and Mercer, 1993) and (Newell *et al*, 1995).

To define stratigraphy, which can be used to identify capillary barriers (and other geologic controls) that may effectively limit the downward migration of NAPL (Newell *et al*, 1995).

To delineate NAPL distribution. NAPL partition into three phases depending on the nature of the NAPL, i.e. into solution, free phase and/or residual. The delineation of mobile NAPL is necessary for the containment of the DNAPL, and it will flow unless it is immobilized in a stratigraphic trap or by hydrodynamic forces (Cohen and Mercer, 1993) and (Newell *et al*, 1995).

To determine the nature and extent of contamination.
The ultimate objective of site characterization is to determine the nature and extent of contamination so that informed decisions can be made regarding remediation. In determining the nature and extent of groundwater contamination, it is important to estimate the hydrogeologic characteristics that influence the contaminant distribution (Cohen and Mercer, 1993).

To determine of migration rates/directions of the mobile phases (Newell *et al*, 1995)

To minimize investigation risk. In performing certain surveys like geophysics, you minimize investigation risk if conclusions can be drawn from initial studies before performing in depth site characterization (Cohen and Mercer, 1993).

To confirm or negate Site Assessment conclusions. Site Characterization also serves the purpose of determining if the initial site conceptual model was correct, and where improvements could be made (Cohen and Mercer, 1993).

To perform a remedy assessment. Site characterization data is ultimately used to evaluate the design and operation of remedial measures at DNAPL sites. Specific data requirements may vary between alternative remedial technologies. Therefore acquisition of site characterization data should be phased and become more focused with respect to remedy selection as the site conceptual model becomes more refined (Cohen and Mercer, 1993) and (Newell *et al*, 1995).

The level of detail and the type of data required for site characterization will be site-specific, partially dictated by the remedial technologies under consideration and practical economic constraints, and often restricted by available characterization technologies. Such limitations include lack of practicable methods for detailed delineation of many parameters of interest including NAPL distribution and saturation and hydraulic conductivity distributions (Newell *et al,* 1995).

6.3 DIFFICULTIES AND CONCERNS REGARDING SITE CHARACTERIZATION

Some difficulties are encountered when performing site characterization. In South Africa, these difficulties are compounded by the fact that certain technologies are too expensive to implement with the South African economy. Other factors that influence the choice of site characterization method is the geology. Fifty percent of South Africa consists of Karoo rocks (Vivier, 1996) which includes a lot hard rock. This does not include granite complexes of the Western Cape which is also hard rock. General site characterization methods may be rendered inappropriate for most of South Africa since the geology mostly comprises a hard rock environment (see Section 6.7 for more detail).

- Free phase DNAPL does not flow in the same way as dissolved phase plumes - DNAPL behavior is only loosely coupled to that of groundwater. Movement of DNAPL is sensitive to capillary properties of the subsurface and the distribution of those properties controls the distribution of DNAPL. Thus a sound knowledge of geologic conditions is more important than knowledge of hydrologic conditions for adequate characterization of DNAPL. To minimize risk of contamination mobilization, it is usually recommended that boreholes not be drilled into DNAPL sites before having detailed the geology of the site by using applicable geophysical techniques. Some sites, however, do not lend themselves to investigation by geophysical techniques, and in such cases it is deemed a better solution to drill and determine the site geology via such means, than to do nothing at all and let the source continue to pollute the subsurface. This is called the outside-in approach.

- DNAPL migrates preferentially through relatively permeable pathways and is influenced by small-scale heterogeneities due to density, capillary forces and viscous forces. The movement and distribution of DNAPL is difficult to determine in fractured bedrock, heterogeneous strata and complex DNAPL mixtures. In South Africa, 50% of the land is Karoo rocks and this includes a lot of hard rock (dolerite). These dolerites with their fractures represent preferential pathways along which organic pollutants migrate, thus hard rock sites should not be treated as porous flow aquifers. In Chapter 7 such a hard rock site is discussed as an example.

- Failure to directly observe DNAPL at a site does not mean it does not exist. Very low aqueous concentrations of DNAPL may be detected at DNAPL contamination sites but these concentrations may already greatly exceed drinking water standards. Here caution must also be taken to analyze the water samples at laboratories with an appropriate (low enough) detection limit, otherwise contamination may also not be picked up.

- The risk of causing DNAPL or LNAPL mobilization must be assessed during site investigation. Conventional drilling technologies have a high potential for promoting vertical DNAPL movement. The appropriate investigation strategy is dependent on site-specific conditions, of which the geology is very important. In South Africa, having hard rock and not sand aquifers like much of Europe where NAPL pollution studies have been performed, drilling methods will differ. Economics also comes into play when deciding the amount, depth and spacing of site characterization boreholes that is to be drilled.

- The more complex the NAPL mixture, the more difficult the characterization of it becomes. For determination of effective solubilities, Raoult's law is technically only applicable if the mixtures consist of structurally similar components. For dissimilar components an analysis error exists, but the error is smaller than a factor of two (Leinonen and Mckay, 1973), which means it can be safely ignored for a site with larger environmental uncertainties. Only the most technologically advanced laboratories (none of which are known in South Africa) may have the analysis techniques available for determining physical properties such as the molecular masses and mole fractions of individual components of a complex mixture NAPL. Also, for a multi-component NAPL, the components with higher effective solubilities are removed from the NAPL first, which in effect changes the effective solubilites of the remaining compounds. This occurs because mass removal occurred and thus changed the molar fractions of the individual components in relation to the mixture. This problem can be addressed by using an effective solubility model (ESM), which has been tested by McKay *et al* (1991) and was found to adequately model and predict the mass removal and change in effective solubilities of the remaining compounds in the mixture.

- Certain hazards may exist during invasive characterization at LNAPL contamination sites. The potential for increasing the vertical extent of contamination should be considered when evaluating drilling and well installation programs. Drilling through mobile LNAPL (e.g., liquids perched on low permeability units above the water table) may result in contaminating deeper intervals. (Newell *et al*, 1995)

- The risk of explosion or fire (API, 1989) may exist at sites contaminated with flammable materials (e.g., most liquid petroleum products). During drilling operations, the material brought to the surface may contain vapors and cause conditions favourable for ignition. NAPL is not only a concern as a fire and explosion hazard, but also with regard to chemical exposure to the driller and sampling crews. Monitoring and mitigation of explosion and exposure risks should be considered when planning field operations. (Newell *et al*, 1995)

- Methods for direct detection of NAPL in soil samples are relatively limited, but visual observation often has been relied upon to make this determination in the field. It may be difficult or impossible to observe NAPLs, which are colorless or clear, heterogeneously distributed in the sample, or present at low saturations (Huling and Weaver, 1991). In order to overcome this problem, centrifugation, examination under ultraviolet light, soil-water separation tests, and addition of hydrophobic dye to preferentially stain NAPL (i.e., Sudan IV) were studied. Of these methods, the use of hydrophobic dye and ultraviolet light examination for fluorescent NAPLs were found to be the simplest and most effective methods. These methods however provide only limited, qualitative information concerning the presence of NAPLs. (Newell *et al*, 1995)

- In geophysical surveys, difficulty might be experienced when the site does not allow geophysical surveys. This is the case where too many buildings, electricity cables and waterlines interfere with geophysical surveys, which industrial sites usually have in abundance. (Newell *et al*, 1995). This could be addressed by performing geophysics outside the site if the site allows it, and extrapolating data to the site. Care should be taken when doing this since site geology can change over small distances, although it is not likely. Site geophysics should be backed up with the drilling of boreholes.

- Well-design criteria can be problematic. In general, conventional construction practices use a filter pack coarser than the surrounding formation to allow entry of the LNAPL. However, research regarding construction materials specifically designed for LNAPL monitoring is relatively limited. Recent studies (Hampton and Heuvelhorst, 1990; Hampton et al., 1991) of filter packs for LNAPL recovery wells indicated traditional design practices may not produce an optimum recovery well in the case of aquifer remediation. In addition, compatibility of materials, including pumps, casing, screens, and bentonite, with the particular LNAPL must be considered (Cohen and Mercer, 1993).

- Non-aqueous phase liquids held in pore spaces under tension as a result of capillary forces are not free to migrate to wells and boreholes. Such contamination may be more extensive than the mobile NAPL and may be a major source for continuing contamination of groundwater. Monitoring wells are not useful for defining this contamination (Abdul *et al*., 1989). Thus, lack of detection of mobile NAPL is not an indication of the absence of such liquids and soil vapor analyses and soil sample analyses should be performed to identify any NAPL that may be adsorbed onto soil particles.

- The NAPL thickness measured in a monitoring well has been reported to typically exceed the NAPL-saturated formation thickness by a factor estimated to range between approximately 2 and 10 (Mercer and Cohen, 1990). Due to this difference, the NAPL thickness measured in a monitoring well has been referred to as an apparent thickness.

- The apparent NAPL thickness measured in the well may be related to the height of the mobile, perched NAPL above the water table (Testa and Paczkowski, 1989). Wells installed through such perched zones, in order to measure the perched NAPL thickness, provide potential pathways for NAPL flow, thus a thorough study of site geology should have been performed before commencing on to drilling through capillary barriers. If the site geology is not well-known, drilling through potential capillary barriers should be avoided.

- A rising or falling water table may promote entry of mobile NAPL into areas not previously contaminated with these liquids or regions of lower NAPL saturation. This results in trapping of additional LNAPL in soil pores with reduction in the volume of mobile NAPL. (Newell *et al,* 1995). Nothing can be done to prevent rise and fall of water table, but the potential spread of pollutants should be a known factor when attempting remediation and when measuring the success of such remediation.

6.4 CHARACTERIZATION METHODS

Non-invasive

Non-invasive methods are used during the site assessment to optimize the cost-effectiveness of a NAPL site characterization program. Specifically, surface geophysical surveys, soil gas analysis, and photo-interpretations can facilitate the characterization of contaminant source areas, geologic controls on contaminant movement and the extent of subsurface contamination (EPA, 1994).

Invasive

After an initial site conceptual model has been developed based on the available information and noninvasive field methods, invasive techniques will be required during site characterization and enable the conduct of risk and remedy assessments.

Invasive techniques should be used with care and in a phased manner so as to improve the site conceptual model (if possible) without causing further pollution to the aquifer. Drilling, well installation and pumping activities present the greatest risk of promoting DNAPL migration during site investigation. Drilling and well installation may create vertical pathways (borehole short-circuiting) for DNAPL movement. If sampling and monitoring procedures and techniques are inadequate, it is possible to drill through a DNAPL zone without detecting the presence of DNAPL. Pumping may increase hydraulic gradients and mobilize stagnant DNAPL, and if pumped in fractured media, may move lateral or downward due to the relatively high fluid velocities. In general, groundwater should not be pumped from an uncontaminated aquifer directly beneath the capillary barrier and overlying DNAPL zone (EPA, 1994).

The general invasive techniques include drilling and test-pit excavation, monitoring well installation for sampling, hydraulic tests and boreholes geophysics (Cohen and Mercer, 1993).

TABLE 6-2 lists different characterization methods which can be employed, with its applicability for use in fractured rock environments and unconsolidated formations. It also gives applicability for delineation of LNAPL and DNAPL, as well as the advantages and disadvantages of each technique. The methods are listed from non-invasive towards invasive, with the invasive methods starting at visual methods, which can be non-invasive (for topsoil samples) towards invasive (samples obtained during drilling).

TABLE 6-1: Different characterization methods, applicability for NAPL and hard rock and advantages and disadvantages								
Method		**Fractured Rock**	**Unconsolidated formation**	**DNAPL**	**LNAPL**	**Advantages**	**Disadvantages**	**References**
Visual field evidence – soil/fluid centrifuge, dye enhancement		✓ Only for topsoil	✓	✓	✓	Direct evidence	Volume not quantifiable	Cohen and Mercer 1993 Pamkow and Cherry 1996
Enhanced visual methods	Shake tests	✓ Only for topsoil	✓	✓	✓	Direct evidence	Volume not quantifiable	Cohen and Mercer 1993 Pankow and Cherry 1996
	UV fluorescence	✓ Only for topsoil	✓	✓	✓	Indirect evidence (commingled souce) Aromatics and PAH's fluoresce	Volume not quantifiable Can have false positives (shells, humic material also fluoresce)	Cohen and Mercer 1993 Pankow and Cherry 1996
	Dye addition	✓	✓	✓	✓	Direct evidence Excellent screening tool	Volume not quantifiable Sudan IV listed as mutagen Soil type / moisture condition may influence accuracy	Cohen and Mercer 1993 Pankow & Cherry 1996

TABLE 6-1: Different characterization methods, applicability for NAPL and hard rock and advantages and disadvantages *(contd.)*

Method		Fractured Rock	Unconsolidated formation	DNAPL	LNAPL	Advantages	Disadvantages	References
Drilling methods	Auger drilling	None	✓	✓	✓	Good in loose soils, rubble heaps Can conduct soil sampling	Cannot penetrate deep if hard rock is encountered near surface Limited quantities of groundwater sampled Limited well construction capabilities	Cohen and Mercer, 1993
	Air Percussion drilling	✓	✓	✓	✓	Most cost-effective method if drilling into hard rock Good quality formation samples Allows yield estimation	Can only recover loose formation Samples reliable but occurs as chips Potential for vertical cross-contamination Air stream requires contaminant filtration	Cohen and Mercer, 1993
	Core drilling	✓	✓	✓	✓	Recovers drilling core Can do permeability tests on drilling core Holes can be drilled at any angle	More expensive drilling method Slow rate of penetration Can lose large quantities of water to fractures	Cohen and Mercer, 1993
Drilling related measurement	Vapour analyses while drilling	✓	✓	Depending on significant release	✓	Indirect evidence if readings of 1000 – 2000 ppm vapor (may infer DNAPL)	Questionable vertical control Water can skew / inhibit volatile detection False positives due to equipment exhaust possible Semi-quantitative Drilling can lead to vertical migration of contaminants	Cohen and Mercer 1993 Pankow and Cherry 1996
	Drilling water analyses	✓	✓	✓	✓	Indirect evidence Can help to avoid drilling through vertical lithologic barriers	Questionable vertical control Concentrations diluted Not representative of surface conditions Some drilling methods do not yield water Drilling can lead to vertical migration of contaminants	Taylor and Serafni 1988, Cohen and Mercer 1993, Pankow and Cherry 1996
Observation wells		✓	✓	✓	✓	Direct evidence if product recovered Indirect evidence if concentrated dissolved phase constituents detected	Difficult to determine NAPL volume & vertical distribution LNAPL outside well not same as observed in well DNAPL may not flow into well	Cohen and Mercer 1993, Pankow and Cherry 1996

TABLE 6-1: Different characterization methods, applicability for NAPL and hard rock and advantages and disadvantages *(contd.)*

Method	Fractured Rock	Unconsolidated formation	DNAPL	LNAPL	Advantages	Disadvantages	References
Test pits	Depending on depth of bedrock	✓	✓	✓	Examine large portion of subsurface area which may be difficult with boreholes Provides most reliable & detailed info on soil & rock along any vertical / horizontal line	Can only penetrate limited depth, potential subsidence after holes are backfilled DNAPL may not flow into pit Difficult to keep pit open under saturated conditions 5	Cohen and Mercer, 1993 US Military, 2001 Pankow and Cherry, 1996
Chemical anaysis – soil, rock, water samples	✓	✓	✓	✓	Direct evidence Vertically continuous samples lead to reliable identification	Lack of reliable sampling methodology Potential for loss of volatiles Improper collection can lead to vertical migration of contaminants	Cohen and Mercer, 1993 Pankow and Cherry (1996)
Partioning interwell tracer tests	✓	✓	✓	✓	Indirect evidence Can be used for volume estimates and evaluation of remediation method efficiency Can detect NAPL saturation	Partition coefficient variability due to differences in NAPL composition can introduce errors in the estimation of NAPL saturation. It is also important to recognize that thin fractures in karst, clays, or crystalline rocks can skew the results due to random migration in fractured media	Jin *et al*, 1995 Annable *et al*, 1998 Nelson *et al*, 1999 Deeds *et al,* 1999 Dwarakanath et al. 1999 Keller *et al*, 2000
Radon flux rates	✓	✓	✓	✓	Indirect evidence based on Rn concentration deficits due to partitioning into the organic phase Passive sampling (opposed to injection)	Logistically difficult Lack of reliable sampling methodology Specialized sampling and analytical procedures required Geological factors may lead to low correlation between Rn and NAPL presence	Semprini *et al,* 1998
Backtracking using dissolved well concentrations	✓	✓	✓	✓	Indirect evidence Extreme temporal variations in dissolved concentrations may indicate that the well is located along the margin of a dissolved plume.	Conditions must be ideal (significant source volume, conditions that impede dissolved contaminant degradation) Active sampling, spacing of monitoring wells, well screen length may dilute concentrations Highly conductive zones can demonstrate lower concentrations in course grained, well flushed materials	Newell *et al*, 1995 Cohen and Mercer, 1993

TABLE 6-1: Different characterization methods, applicability for NAPL and hard rock and advantages and disadvantages *(contd.)*

Method		Fractured Rock	Unconsolidated formation	DNAPL	LNAPL	Advantages	Disadvantages	References
Down the hole geophysics	Electrical resistivity	✓	✓	✓	✓	Evaluate clay content and fracture density, as well as fluid conductivity. High resistivity may reflect NAPL presence	Can not be used with PVC or steel casing, can only be used in uncased holes. Can not be used in the unsaturated zone. Well diameter must be greater than 2 inches	Cohen and Mercer, 1993 EPA (b), 1997
	Natural gamma	✓	✓	✓	✓	Can determine clay content of formation (which may act as NAPL capillary barriers). Can be used in uncased and cased holes.	Well diameter must be greater than 2 inches	Cohen and Mercer, 1993 EPA (b), 1997
	Neutron-neutron	✓	✓	✓	✓	Provide estimates of moisture content in vadose zone, total porosity in saturated zone and rate of fluid infiltration	Well diameter must be greater than 2 inches	Cohen and Mercer, 1993 EPA (b), 1997
Cone Penetrometer Test (CPT) methods	CPT methods (Laser Induced Fluorescence)	✓	✓	✓	✓ Indirect evidence	Applicable for LNAPL delineation Indirect DNAPL evidence - on fluorescence of commingled materials Depth discreet signals Good screening method with high resolution	Limited by lithology False negatives and positives possible Semi-quantative, requires confirmation samples Pressure/ heat front may force droplets away from window	Kram, 1998 Kram *et al*, 2000 ITRC, 2000
	CPT methods: GeoVis	✓	✓	✓	✓	Direct evidence based on video image processing Data easy to interpret in light-colored soil matrix	Limited by lithology Rate of data correlation limited by visibility Transparent NAPL droplets not visually detectable Pressure / heat front may force droplets away from window	Lieberman and Knowles 1998, Lieberman *et al*, 2000
	Flexible liner underground everting (FLUTe membrane)	✓	✓	✓	✓	Direct evidence Can be deployed using CPT Good screening method with good resolution	Qualitative, Requires confirmation sampling, May be difficult to apply in consolidated materials	MSE, 2000

6.5 WELL, SOIL AND POLLUTANT TESTS

Several tests must be conducted to determine parameters for the conceptual model, which are listed in the tables below for:

- unconsolidated deposit
- bedrock; and
- contaminant characteristics, that are to be determined.

The following unconsolidated deposit information (**TABLE 6-2**) may be determined during site investigations (Environment Agency, 2003):

TABLE 6-2: Unconsolidated deposit information needs

Parameter	Type of test for parameter determination	Example of use of information
Porosity	Laboratory determined, tracer test	Plume velocity, diffusion calculations
Dry bulk density	Soil analysis – laboratory determined	DNAPL threshold concentration calculations
Fraction of organic carbon	Soil – lab determined, see Chapter 4, Section 4.4.3	Plume velocity calculation, DNAPL threshold calculation
Hydraulic conductivity	Hydraulic test – see Chapter 4, section 4.4.1 for textbook values	Plume velocity calculation, design of extraction wells
Displacement pressure	Calculated from hydraulic tests	Pool height calculations
Bulk retention capacity	0.25-3% depending on geology, type of release	DNAPL mass estimate
Contact Angle	Laboratory determined / Macro-photography, see Chapter 4, Section 4.3.5	Refinement of conceptual model on DNAPL mobility
Hydraulic head distribution	Laboratory determined, tracer test	Directions of groundwater flow and velocity of groundwater
Bedding structures	Visual inspection of drill core	Directions of DNAPL migration
Spatial extent of NAPL source zone	Historical information on dumping area / Estimated from free phase NAPL encountered in wells	Guide remedy selection and design
Spatial extent of plume	Groundwater analysis of organic compounds	Guide remedy selection, risk analysis

Bedrock properties to determine during site investigations are given in **TABLE 6-3** (Environment Agency, 2003):

TABLE 6-3: Bedrock information needs		
Parameter	**Type of test for parameter determination**	**Example of use**
Matrix porosity Matrix dry bulk density Matrix fraction organic carbon	Core analysis Lab determination Soil – laboratory analysis, see Chapter 4, Section 4.4.3	Diffusion calculations Estimate remediation timeframe Estimate retarded plume velocity
Orientation of major fracture sets	Visual inspection of drilling core; down-the-hole cameras	Determine direction of plume migration Directions of DNAPL migration
Fracture spacing	Visual inspection of drilling core; down-the-hole cameras	Diffusion calculations
Fracture porosity	Tracer test, laboratory determined	Plume velocity calculation
Bulk rock hydraulic conductivity	Hydraulic tests	Plume velocity calculation Design of extraction wells
Hydraulic head distribution	Water level measurements, hydraulic tests	Directions of groundwater flow and velocity of groundwater
Bulk retention capacity	0.25-3% depending on geology, type of release	DNAPL mass estimate
Contact angle	Laboratory determined / Macro-photography, see Chapter 4, Section 4.3.4	DNAPL-rock-water wetting relationship
Spatial extent of NAPL source zone	Historical information on dumping area / Estimated from free phase NAPL encountered in wells	Guide remedy selection
Spatial extent of plume	Groundwater analysis of organic compounds	Guide remedy selection, risk analysis

Contaminant characteristics to determine during site characterization (Environment Agency, 2003) are given in **TABLE 6-4**:

TABLE 6-4: Contaminant characteristic needs		
Parameter	**Type of test for parameter determination**	**Example of use of the information**
NAPL density	Laboratory determination – see Chapter 4, section 4.3.1, single component densities can be found in Appendix A, Data Set 1 and 2	DNAPL mobility and pool height calculations

TABLE 6-5: Contaminant characteristic needs *(contd.)*		
Parameter	**Type of test for parameter determination**	**Example of use of the information**
NAPL viscosity	Laboratory determination – see Chapter 4, Section 4.3.2, single component viscosities can be found in Appendix A, Data Set 1 and 2	Determine if DNAPL could still be moving Design of NAPL recovery system
NAPL component composition	Laboratory determination	Effective solubility calculations Predict future composition of the plume
NAPL-water interfacial tension	Laboratory determination – see Chapter 4, section 4.3.3, single component interfacial tensions can be found in Appendix A, Data Set 1 and 2	Determine importance of capillary forces Pool height calculations
Organic carbon partition coefficient (Koc)	Laboratory determination – see Chapter 4, section 4.4.2	Determine degree of aqueous phase sorption and rate of plume migration
Contaminant half-life	Single component half-lifes can be found in Appendix A, Data Set 1 and 2, mixed component half-life: laboratory determined	Determine degree of degradation and rate of plume migration
Date and volume of release	Historical information	Estimate depth of DNAPL migration - is DNAPL still moving?
Potential NAPL release locations	Historical information	Help guide monitoring well placement

The application of the site characterization methods listed in **TABLE 6-1**, as well as the well, soil and pollutant tests listed above will be demonstrated in Chapters 7 and 8.

6.6 SITE CHARACTERIZATION OF FRACTURED ROCK

South African geology:

Geology plays an important role in the choice of characterization methods (e.g. choosing the correct drilling methods), the effectiveness of characterization and the options that are available for remediation.

As has been highlighted, hard rock makes up a large part of South Africa’s geology. Hard rock has one inherent feature, which are fractures. In **FIGURE 6-1**, fractures, undifferentiated lineaments and dykes have been mapped for South Africa (Data obtained from Council for Geoscience database, 2004).

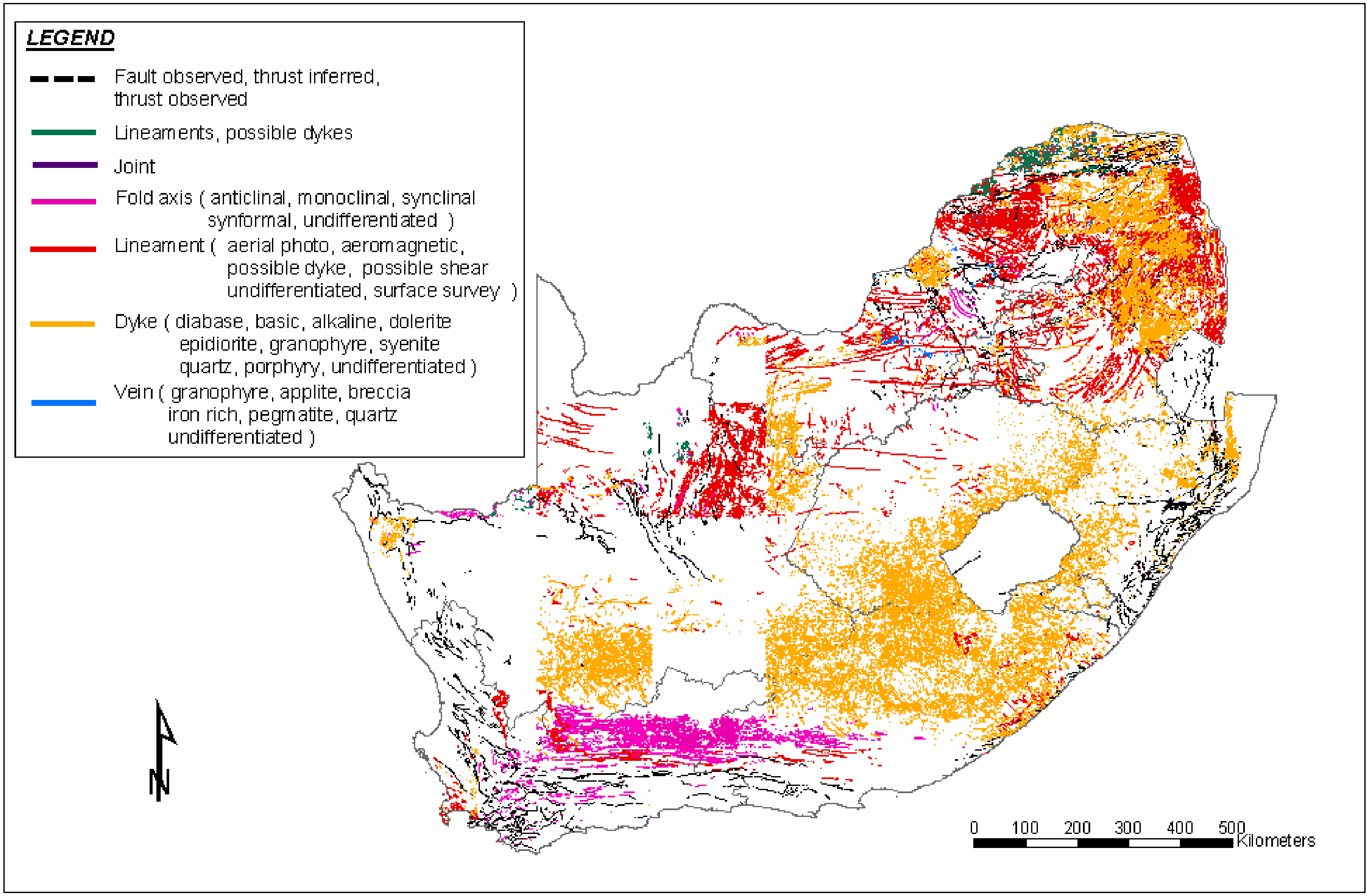


Figure 6-1 (Fracture lineaments South Africa) – (Council for Geoscience database)

From the map the following can be seen:

- Lineaments (possibly dykes) cover the whole of South Africa (these can be fractures of structures) – seen in red on **FIGURE 6-1.**
- Dykes cover almost the whole of the Karoo basin (Karoo, Northern Cape), as well as areas of Limpopo and Namaqualand. Fractures are associated with these intrusions. The dykes can be seen in orange on **FIGURE 6-1.**
- Fold axis has also been plotted to indicate the position of the folds, since fractures are associated with the incompetent rocks of the folds (in purple on **FIGURE 6-1**).
- The center of South Africa has not been fully mapped as yet, but comprises the Karoo rocks which are associated with dykes.

Fractures are especially problematic for characterization and remediation of NAPL. Hard rock poses problems for modeling aquifer conditions and several models have already been developed to accurately predict groundwater (and possibly NAPL) flow in hard rock. Apart from prediction of flow, there is also prediction of contaminant spread and attenuation, where risk assessment comes in.

Over the past two decades, there has been increasing recognition that geologic complexities pose some of the greatest challenges to site characterization and groundwater restoration (EPA, 2001). Fractured rock sites are among the most complex because of their considerable geologic heterogeneity and the nature of fluid flow and contaminant transport through fractured media. Relative to most unconsolidated deposits, characterization of contaminant migration in fractured rock usually requires more information to provide a similar level of understanding. The complexity of contaminant source conditions also makes remediation more difficult (EPA, 2001).

Type of drilling method to be used in fractured rock environments:

Geological characterization at fractured rock sites includes the use of conventional techniques such as outcrop mapping, fracture trace analysis, drilling, coring, and, more recently, increased use of borehole geophysics. *Drilling boreholes remains the principal means of geological characterization and, because it is generally slow and expensive, contributes significantly to characterization costs* (EPA, 2001).

Several drilling methods exist. For soft overburden, cone penetrometer technology (CPT) can be used, but as soon as hard rock is encountered, this technology is inefficient. The potential distribution of NAPL in the overburden can however be assessed. Currently the Council for Geoscience is the only company providing CPT in South Africa. CPT is more advanced than auger drilling since a hollow stem core is advanced into the ground and a soil core is retrieved, whereas Auger mixes up the soil sample. Real time data is this obtained and precision sampling can be performed. Porosity tests can be performed on these cores. Drilling in hard rock can be done with core drills or air percussion, as well as sonic drills (very expensive).

In the United States of America (USA), core drillings are usually used in order to determine fracture sizes, directions, and if water flows through the fractures (if fracture surfaces are weathered, water flows through the fractures). However, the following problems are experienced with core drilling:

- It is very expensive to collect oriented cores to determine the dip and strike of the fracture features and it may also be very difficult to ascertain if the drilling itself does not cause the fractures.
- The presence or absence of fracture oxidation and weathering, and fracture fill or coatings, can provide direct indications of likelihood of groundwater flow. However, fracture zones, which are of most interest to investigators, are poorly recovered from core samples.
- Zones of potential importance for groundwater flow frequently correspond to rubble zones or lost sections of core.
  (EPA, 2001)

Workshop discussions held in the USA, reflected a current debate over the cost-effectiveness of obtaining core during drilling. In response to the workshop questionnaire, almost all (94%) of respondents indicated they had used coring in characterization of fractured rock sites. The survey did not indicate how important they rated core analysis for characterization, the percentage of holes that were cored, or whether their reliance on it had changed over time. (EPA, 2001)

In South Africa, air percussion drilling is usually used to characterize the groundwater regime and determine the type of rock. Core drilling is too expensive a technology to use. Fractures are inferred from water strikes and down-the-hole videos can determine fracture dip and size. **FIGURE 6-2** is an example of a fracture photograph taken in a borehole with a down-the-hole video camera (Credit: IGS and DWAF (2000)). The yellow arrow shows the position of the fracture.

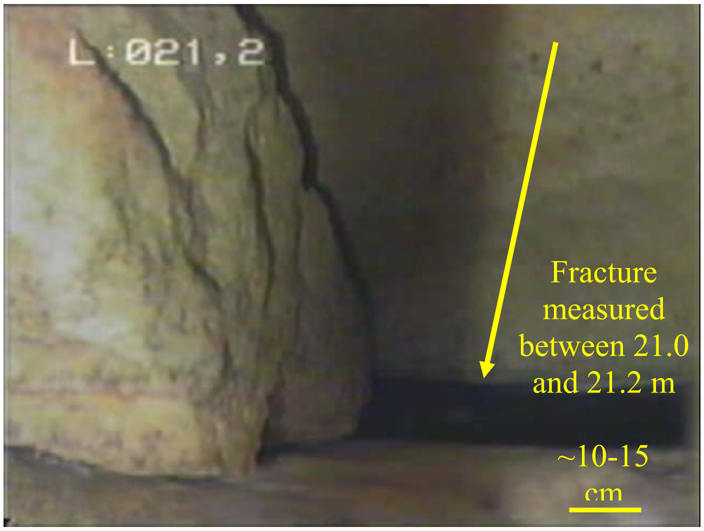


Figure 6-2 (Fracture photo)

Taking into account the costs involved in core drilling, that core loss generally occurs at the important fracture zones, and that similar information can be obtained by using air percussion drilling and down the hole geophysics / borehole video's, drilling holes in fractured rock in South Africa with air percussion, seems to be the most cost effective drilling method.

Practical examples of the determination of various parameters i.e. fracture aperture, entry pressures and pool heights which are important for fracture flow, will be given in Chapter 7, where the case study is presented.

6.7 CONCLUSIONS AND RECOMMENDATIONS

The following conclusions can be drawn and recommendations made:

- Money, legal framework, specific negotiations with authorities, and specific site characteristics (e.g. geology, land-use) all determine the Site Characterization approach. Drilling techniques that may be viable in the United States of America or Europe may not be economically viable in South Africa.

- Several NAPL characteristics cause characterization difficulties and may compound characterization costs, which may include amongst others more expensive drilling techniques, safety precautions that need to be implemented during drilling, certain materials that need to be used during well-installation because of the corrosive nature of NAPL, certain sampling precautions that need be taken to ensure that volatile organics are not lost during sampling etc. Cost savings on some of the above-mentioned factors may lead to vital characterization and conceptual model mistakes, and is not recommended.

- Two types of characterization methods exist: Non-invasive and invasive. By first employing site-applicable non-invasive methods of characterization, one may lower the risk of possible wider NAPL contamination in the aquifer and this may also imply large cost-savings in that the choice and use of certain invasive methods may be more applicable to the site. This, in turn implies cost-savings on later re-characterizing the site due to poor choices made on characterization technologies that does not answer the questions that need to be answered. The non-invasive phase may be seen as a compulsory predecessor of the invasive characterization phase.

- An outside-in approach in terms of site characterization must always be followed in order to lower the possibility of spreading contamination during drilling and sampling programmes, especially in a hard rock environment.

- Geophysical techniques are becoming more useful as technologies advance and must be considered during site characterization since it would implicate large cost savings. See section 6.5.

- It must first be determined if the site geology and suspected NAPL pollutant lends itself towards soil vapor analysis, before this type of analysis is performed, as can be seen in **TABLE 6-1**. If this analysis is performed indiscriminately, it may implicate money wasting since these surveys do not always yield useable information, if any. This technology is more applicable to LNAPL sites than to DNAPL sites.

- The effectiveness of different characterization methods must first be determined for a specific site before it is employed, since ineffective characterization methods could effect unnecessary expenditure.

Chapter 7

Impact Assessment

7.1 INTRODUCTION

Impact assessment is performed before risk assessment, and usually forms part of site assessment and site characterization. During impact assessment the extent of pollution is determined, where the extent is measured against a legal boundary, be it a compliance boundary (e.g. a river or groundwater users) or the perimeter of the site. An aspect and impact register is also drawn up, highlighting all possible aspects that can contribute towards the pollution, and the impacts that these aspects will have on the site and the receptor.

In order to explain impact assessment, a hypothetical example will be given, using real data, but applied on a generic site. This is done because NAPL pollution is a very sensitive issue in South Africa. Real data is used to make the example as applicable as possible to South African circumstances. A site assessment and site characterization will be performed on the fictitious site before doing an impact assessment.

7.2 CASE STUDY

SITE DESCRIPTION AND BACKGROUND INFORMATION:

Background information:

No coordinates will be given for this site. A fictional north is given for the site and an ortho-photomap has been compiled from different photographs for the site. This serves as a base map. No topographical highs were allocated for the site, but a proposed groundwater flow direction is given for the site, assuming that the normal groundwater flow follows the topography (Bayesian principle) (Van Sandwyk *et al*, 1992). The red arrow indicates the groundwater flow direction. See **FIGURE 7-1.**

Site description:

Although the site is located in a typical industrial area, a residential area also occurs southeast of the site, which was developed by the specific industry to house its employees. Another industry occurs northeast of the site and directly east of the site is an open veld area. The legal boundary of the site (perimeter) is given in blue. A natural groundwater divide runs along the western boundary of the site, which is shown in purple. All these can be seen in **FIGURE 7-1**.

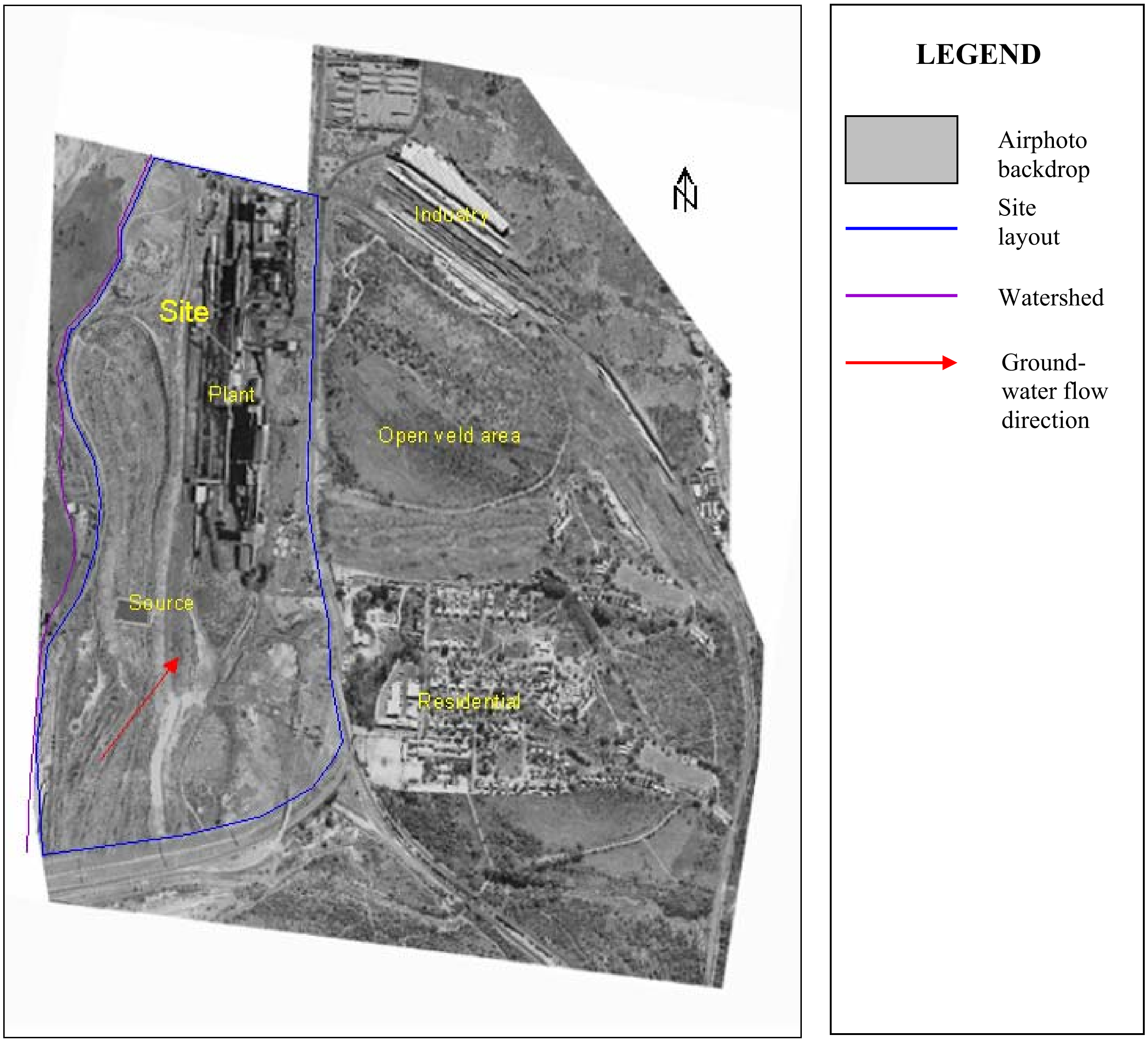


Figure 7-1 (Site map)

7.2.1 Site assessment

During the site assessment, the following actions were performed:

- Site visit
- Obtaining all relevant existing information (reports and data, e.g. plant and site layout) from the industry
- Obtaining an orthophoto of the area
- Performing a hydro-census to identify all possible receptors in the area (no river is near the site), during which samples were taken from the wells to be analyzed by an accredited laboratory. Water levels could not be measured at these boreholes since they were both equipped with pumps. The boreholes positions were taken with a global positioning system (GPS) (correct

within 10m) to plot them on the basemap. Hiring a surveyor to survey two boreholes proved too expensive and was only used at the end of the drilling phase to obtain the coordinates of the drilled boreholes corrected up to 1m.

- Obtaining the local 1:50 000 geology map of the area to plot the plant and site areas and existing boreholes on.
- Performing a geophysical survey on the southern part of the site using a proton-magnetometer – which was the only area permitting geophysics. The other areas had too much cultural interference.
- Siting the initial boreholes
- Drilling the initial boreholes (30m deep) and taking GPS coordinates. No free-phase NAPL were encountered in any of these boreholes and no oily substances were smelt during drilling. The initial drilled boreholes consisted of boreholes B1-B7.
- Soil samples were taken from the following boreholes (which are in the vicinity of the pollution source): B5 – B7. It was subjected to UV fluorescence, but no fluorescence was observed.
- After two weeks, the stabilized water levels were taken in the newly drilled holes, and the boreholes were logged with an YSI 600XLM multi-parameter profiler (in boreholes that encountered only water and no NAPL). The YSI 600XLM measures electrical conductivity (EC), dissolved oxygen (DO), temperature and pH. The sampling depth for inorganic variables was inferred from the EC profile, where a peak in the EC measurements usually indicates flow from the fracture zone. The inorganic variables analyses and results will not be discussed since this does not form part of the objective of the thesis.
- Stratified sampling depths were chosen after the multi-parameter profile data were processed.
- Inorganic groundwater samples were taken from the drilled boreholes using a stratified sampler. (Inorganic analyses will not be described and analysed in this chapter, since the thesis focus is on organic pollution. Inorganic analyses are however, as important as organic analyses in a impact assessment and risk study).
- Water samples for organic analyses were taken from boreholes B1 – B7 at the stratified depths (which will be called top, middle and bottom).
- These samples were analysed for volatile organic compounds (VOC) at the top, voc and semi-volatile organic compounds (SVOC) in the middle and SVOC at the bottom of the wells. The analyses results are shown in **TABLE 7-4**.
- An initial conceptual model was drawn up, which was used to plan the site characterization phase.

During the hydro-census, which was performed as part of the site assessment, the following receptor boreholes were identified:

R1	A residential borehole in the employee residential area used for watering the garden (no domestic use was reported).
R2	A regulatory authority monitoring borehole downstream from the low-impact wood re-working industry. The industry obtains it wood from a nearby pine plantation.

No VOC screening or soil gas analyses were performed since it was deemed an unnecessary expenditure. The type of NAPL dumped on site is known to be coal tar type NAPL (long chain hydrocarbons and PAH's), as gathered from industry process engineers on site. These contaminants do not partition adequately into the gas phase to be detected under normal soil gas analysis circumstances (EPA, 1994). In addition VOC screening membranes give only a flux count related to concentration but which can not be extrapolated directly to concentration. Membrane porosity also usually differs from one membrane to the next, giving inconsistent flux ratios.

Regional geology:

The regional geology on and around the site was determined to be the Marico Diabase Suite. The Marico Diabase Suite, which is probably related to an early intrusive phase of the Bushveld Complex, comprises three distinct lithological types:

> *Maruleng Diabase*: dolerite dykes and sills, often of noritic composition
>
> *Lydenburg Diabase*: hornblende-bearing dolerite dykes and sills often of gabbroic composition
>
> *Wanhoop Diorite*: dioritic dykes of calc-alkaline affinity
>
> Informally and collectively referred to as Transvaal diabase, these rocks are intrusive into all horizons of the Transvaal Sequence, mainly on the southern side of the Bushveld Complex and more particularly on the southeastern side. The Maruleng Diabase sills are largely confined to the margin of the Bushveld Complex, while the Lydenburg Diabase occurs farther out.

The regional geology can be seen in **FIGURE 7-2** below.

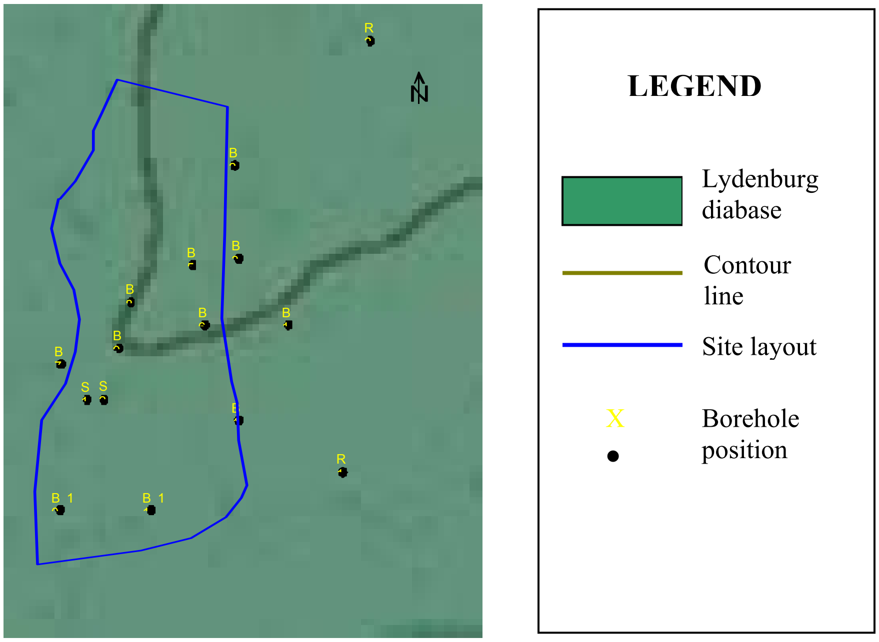
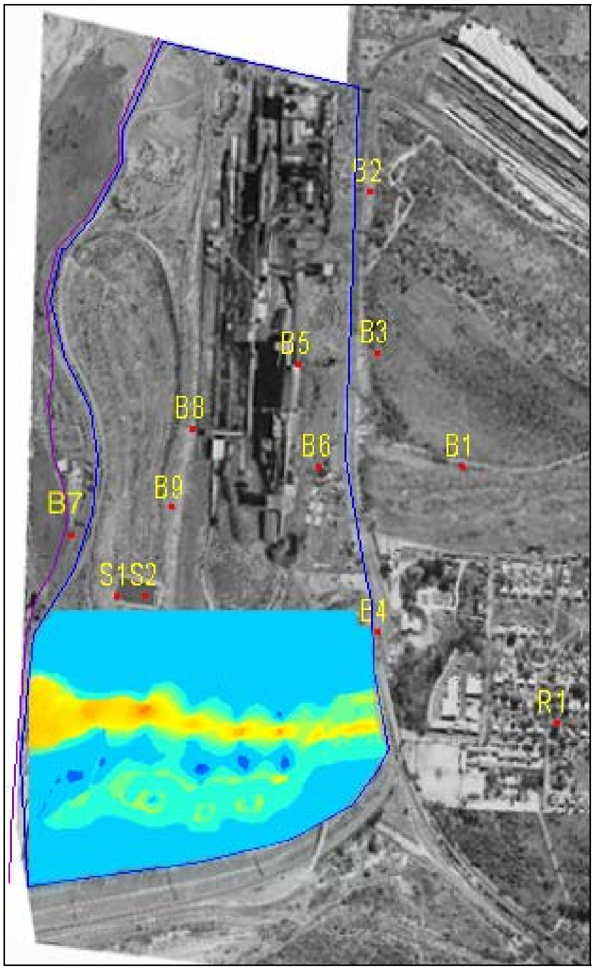


Figure 7-2 (Hypothetical Regional Geology)

Local geology:

During the magnetic survey seven lines were walked in a grid from north to south in the southern area of the site, which was the only area permitting geophysics. Cultural interference excluded the use of a magnetometer in the northern part of the site. One anomaly was identified which is shown in **FIGURE 7-3** below. Other geophysics was not employed since a magnetometer is effective enough and a cost-effective method for determining the existence of diabase dykes. The magnetometer was not used to infer pollution plumes as it would have been ineffective for such an application.



LEGEND

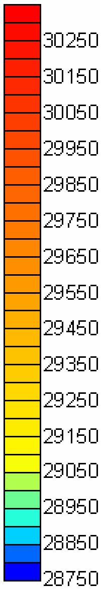
▨ Airphoto backdrop

— Site layout

— Watershed

X ● Borehole position

The magnetic anomaly that was identified, was contoured using Surfer. The colour scale is shown below (given in nanoTesla):



It can be seen that red represents the highest anomaly and blue the lowest.

Figure 7-3 (Hypothetical Local Geology)

The following boreholes were drilled during the site assessment, following the outside-in approach:

B1 Drilled outside the site to the east in order to see the extent of the pollution plume, since no significant pollution was picked up in during the analyses of the sampled hydro-census boreholes.

B2 Drilled to the north on the eastern perimeter of the site.

B3	Drilled in the middle of the eastern perimeter.
B4	Drilled in the south of the eastern perimeter and placed so as to intersect the magnetic anomaly, which was thought to be a dolerite dyke. This was confirmed during drilling.
B5	Drilled at the plant to pick up groundwater contamination from oil runoff from the plant operations, as well as the pollution plume from the source.
B6	Drilled between the plant and the perimeter to determine the contamination concentration at that point.
B7	Drilled as background hole.

Only one borehole has been drilled along the western perimeter of the site to serve as background hole, since the incline on the western boundary is too steep and the terrain too inaccessible to allow a borehole. A power line also runs along this boundary and the borehole could not be drilled too close to the power line according to drilling safety regulations. No boreholes have been drilled west of the water divide since water divides serve as no-flow boundaries for groundwater.

After drilling these boreholes, samples were taken and analyzed for organic constituents, which were are listed in **TABLE 7-4.** During the site assessment phase, an initial conceptual model was compiled from the current data. Geophysics could only be performed in the south of the site due to too much cultural interference in the north of the site. A magnetic survey was performed on the site because the area was too small an area to investigate to justify the hiring electromagnetic equipment (EM). Magnetic surveys also prove to be an adequate delineation tool in hard rock areas. The weathering was observed to be to a depth of approximately 25 m, where the diabase intrusion was encountered, which has associated fresh fractures in the centre of the intrusion.

The initial conceptual model was derived from the initial site investigations and is shown in **FIGURE 7-4** below:

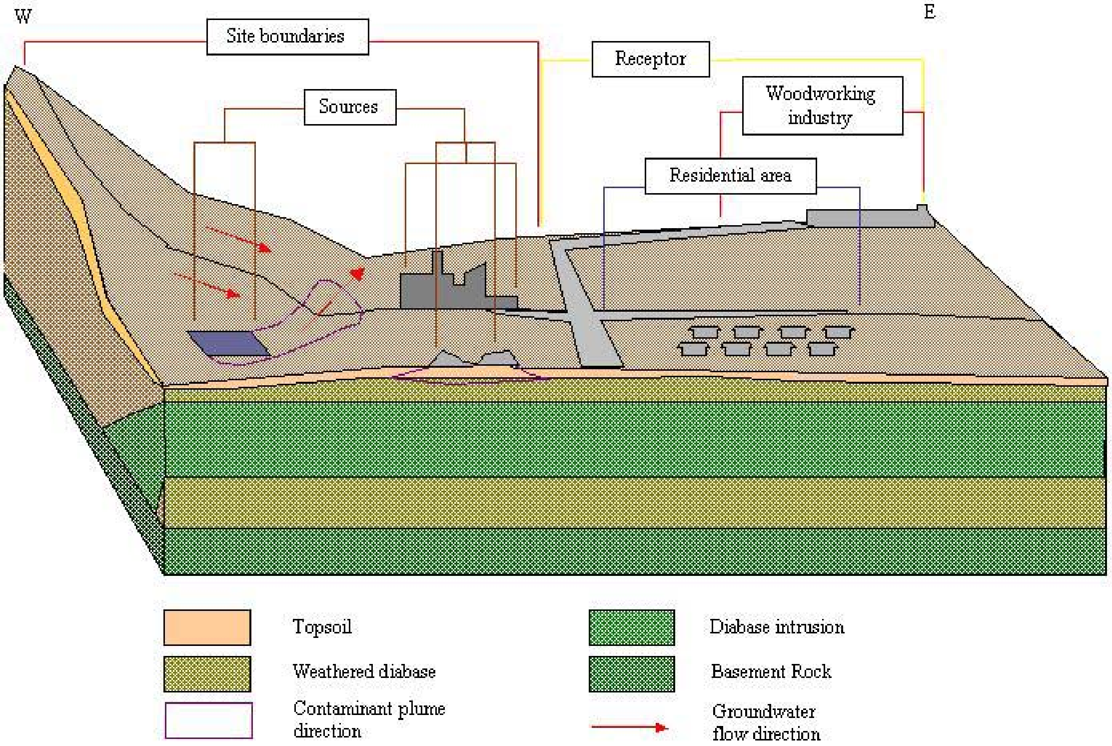


Figure 7-4 (Initial site conceptual model)

From **FIGURE 7-4** it can be seen that it is thought that the contaminant plume moves with the groundwater flow direction, the diabase intrusion has only been drawn in and it is still uncertain at this stage whether the intrusion dips towards the south, although it is suspected from the magnetic survey. The thickness of the sill is also unkown.

7.2.2 Site Characterization

During the site characterization phase the following actions were performed:

- Site selection and drilling of the following boreholes:

B8	Drilled as a plume interception borehole
B9	Drilled as a plume interception borehole
S1	A shallow hole drilled near the source (up-gradient of the source)
S2	A shallow hole drilled down-gradient of the source

- Soil samples were taken every 1m during the drilling of the following boreholes: B8-B9 and S1-S2. These were subjected to UV-fluorescence. B8 showed minimal fluorescence, but B9, S1 and

S2 showed fluorescence at depths of approximately 17-19 m. Photographs were taken of these and the results are shown in Section 7.2.2.1.1.

- After ascertaining that the above-mentioned boreholes did indeed contain PAH's at depths 17-19m, the soil samples from depths 15-22 m of all the drilled boreholes were send for laboratory analyses and the results are shown in Section 7.2.2.1.2. Calculations were also performed on these soil sample analyses results in order to confirm whether or not NAPL is present.
- Water samples for organic analyses were taken from boreholes B8 and B9 at the stratified depths (which will be called top, middle and bottom). An in-detail description of the drilling, construction and sampling will be given below (See: *Notes on the drilling, well construction, well development and sampling*).
- These samples were analysed for VOC at the top, VOC and SVOC in the middle and SVOC at the bottom of the wells. The analyses results are shown in **TABLE 7-4**.
- Shallow holes (S1 and S2 – each 15m deep) were drilled upstream and downstream of the source to determine if any free phase NAPL is present, at what depth and what the consistency of the NAPL is.
- Water samples were collected from the shallow holes at depths 3, 7, and 12m and were analyzed for organic and inorganic constituents.
- Soil samples were taken at 1m intervals from all of the drilled boreholes.
- The soil samples were submitted to UV fluorescent light in order to determine whether any polycyclic aromatic hydrocarbons were present. From the regional geology of the area, it was ascertained that the deposits in the area were mostly weathered volcanic rock from the Marico Diabase Suite and that no shells would be present that would give a false positive.
- Site selection of the following boreholes:

B10	Drilled close to the magnetic high on the medium anomaly to see if the dyke dips towards the south, for initial groundwater sampling (to determine the extent of the plume) and for future monitoring.
B11	Also drilled for the same reasons as above.

- Drilling of boreholes B10 and B11. It was decided to drill these boreholes after geophysical interpretation.

Notes on the drilling, well construction, well development and sampling:

Drilling:

The wells were generally drilled up to a depth of 30m in order to by-pass the weathered zone and get a fair picture of the geology. It was decided that where NAPL was intercepted, drilling would be stopped in order to minimize the downward migration of NAPL to lower aquifer stratum (as was encountered in borehole S2, where NAPL was encountered at 12m). If an aquitard was encountered, drilling was also stopped on this aquitard, for the case where NAPL could have been encountered higher up but was not detected. Drilling could be done through aquitards if a telescoped drilling approach is followed, where each aquifer unit is sealed off. It was however deemed too expensive an approach to follow, and geological and dissolved phase contamination representative of the different aquifers could be obtained from the monitoring wells further away from the source zone. No aquitards were encountered during drilling.

Construction:

The monitoring well was installed as follows: The hole diameter was wider than the casing diameter in order to install a sand pack around the casing. The gravel (sand) size was coarser than the surrounding geological material in order to facilitate NAPL entry into the well. The well was fitted with slotted casing over the whole length of the well (as to allow variable depth sampling for VOCs and SVOCs), and to at least 2 m above the water table to allow for seasonal fluctuations. The well screen was fitted to the bottom of the wells in order to be able sample NAPL that may be pooled on an aquitard but may not be of sufficient volume to rise up to the well screen level. A cement basket and sump was fitted to the bottom of the well in which DNAPL must accumulate (see Figure 7-5). This was also done to prevent NAPL from leaking out of the borehole, which will render the borehole as a contamination conduit for deeper aquifers. Stainless steel casing was used since PVC and Teflon casing are not as strong and as resistant to organic weathering and could introduce minute concentrations of artificial organic contaminants to the groundwater.

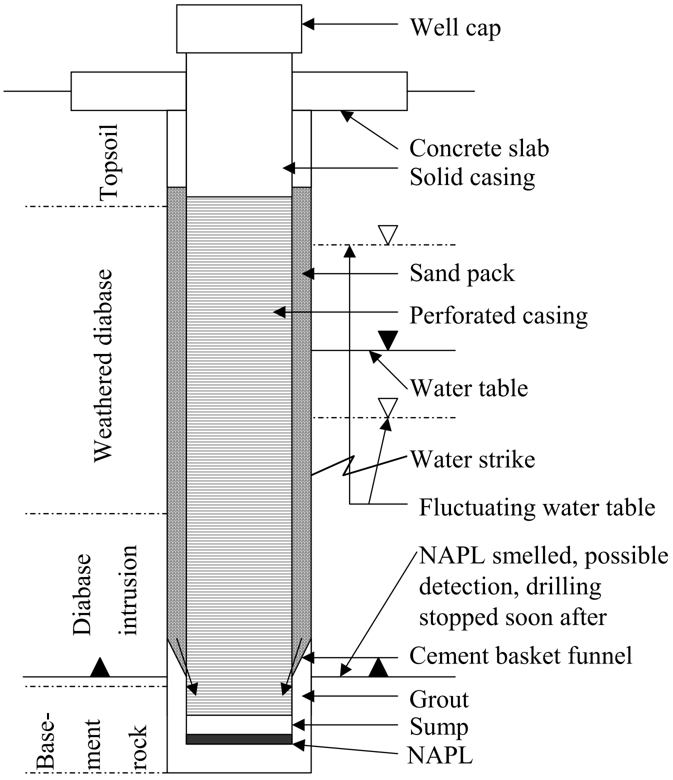


Figure 7-5 (Well construction and lithological log)

Well development:

Well development involves the cleaning of the well from drilling chips etc. so as to open water bearing features. Well development was limited to the outside holes (far from the source) and was totally avoided in the wells were NAPL was encountered, since development of these wells could introduce NAPL contamination to aquifer areas previously uncontaminated.

Sampling:

Samples were taken at three depth intervals, VOCs at the top, SVOCs and VOCs in the middle and SVOCs at the bottom. The sample order is also the order of parameter volatilization sensitivity. These samples were taken with stainless steel bailers with a steel ball valve to ensure that high density NAPL does not leak out. Since disposable bailers are usually PVC and Teflon, which could introduce artificial organic contaminants, they were not used. The density of PVC and Teflon is also such that high density DNAPL may leak out of these bailers (PVC has a density of 1.4 g/cm3 and Teflon 2.2 g/cm3) (Pankow and Cherry, 1996). In addition, PCV and Teflon bailers are much harder to decontaminate in comparison with stainless steel (Parker and Ranney, 1997). A new segment of line was used on the bailer for each sample taken. With detection limits of parts per million and even parts per billion, extreme care was taken to de-contaminate all equipment between every sampling event. The EPA region IV procedure (EPA (b), 2001) for cleaning of stainless steel bailers and other sampling equipment was used:

1. Rinse the equipment several times with pesticide-grade acetone to remove oil/grease (This step is only necessary with hard-to-remove organics).
2. Wash equipment thoroughly with soap and hot tap water using a brush or scrub pad to remove any particulate matter from the surface.
3. Rinse equipment thoroughly with hot tap water.
4. Rinse equipment thoroughly with analyte free water

Once sampling has been finished, repeat steps 1 to 4 and follow up with steps 5 and 6 described below:

5. Rinse equipment thoroughly with solvent and allow to air-dry for at least 24 hours
6. Wrap equipment in one layer of aluminum foil. Roll edges of foil into a “tab” to allow for easy removal. Seal the foil wrapped equipment in plastic and label.

Samples were collected in brown glass containers (to prevent degradation by UV rays from light) and the sample bottle caps were lined with Teflon. Equipment blanks were taken to check the effectiveness of equipment decontamination procedures.

Constituent analyses:

No screening (NAPL ribbon sampling, OVA analyses) was performed but it was rather decided to spend the money on a GC-MS scan of samples taken from all boreholes in order to outline possible contaminants. This was also done because the associated contaminants of a mixed NAPL tar are highly varied and it was aimed to identify as much organic contaminants as possible.

No free phase NAPL was encountered in any of the B-boreholes. During the drilling of borehole B9, an oily substance was smelled and drilling was stopped at 20 m for fear of creating a short-circuit for undetected NAPL to lower aquifer levels. Free phase NAPL was not encountered in hole S1, but in hole S2, at a depth of 12 m, free phase NAPL was encountered, of which a sample was taken which was sent off to an overseas laboratory for the determination of essential parameters, which will be given in Section 7.2.2.1.4**.** Drilling was stopped at 12 m when the free phase NAPL was encountered, in order to prevent further aquifer contamination.

7.2.2.1 Analyses results

7.2.2.1.1 Soil sample UV fluorescence

UV fluorescence is one of the visual detection screening tools to determine the presence of NAPL in an aquifer, which can be performed to get an idea of possible polluted sites before groundwater analyses become available from the laboratory. The technique is cheap and can give relatively good results.

The soil samples that were subjected to UV fluorescence and showed fluorescence are assumed to contain polycyclic aromatic hydrocarbons sorbed onto the soil. In **FIGURE 7-6** and **FIGURE 7-7**, UV fluorescence of samples from borehole S2 can be seen.

Figure 7-6 (Soil samples under normal light)

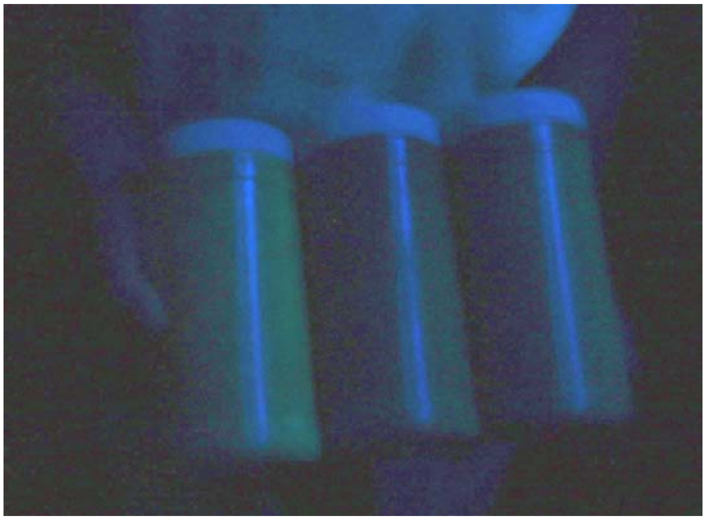


Figure 7-7 (Soil samples under UV fluorescent light)

The samples have been taken at depths 17m, 18m and 19m, which represent the middle of the aquifer. The 17m sample is the leftmost and the 19m sample the rightmost sample. It can be seen that the sample at depth 17m shows the highest fluorescence. The fluorescence of the chosen boreholes have been mapped in this way and the results can be seen in **TABLE 7-1**.

TABLE 7-1

	B8	**S1**	**S2**
Depth	16	16	16
	17	17	17
	18	18	18
	19	19	19
	20	20	20

Very low fluorescence
Medium fluorescence
High fluorescence

It could thus be concluded that organic pollution should most likely be picked up at boreholes, S1, S2 and B8. However, the possibility of picking up pollution at other boreholes is not excluded. Based on these findings, the depths for laboratory soil analyses were chosen, which was 15-22m.

7.2.2.1.2 Laboratory results of soil samples

Soil samples taken from boreholes B1-B7 (taken during the site assessment phase); from boreholes B8-B9, S1 and S2 (taken during the site characterization phase) and from boreholes B10 and B11 (drilled at the end of the site characterization phase) were send to a soil analyses laboratory for analyses of the presence of organic constituents. Wide mouth bottles with Teflon lined lids were used for the soil samples, and these were filled up to leave as little head-space as possible, which would reduce loss of volatiles (Minnich, 1993). The samples were stored at 4°C and sent to the laboratory for analyses. The low temperature decreases the loss of volatiles during opening of the jars for analyses (Minnich, 1993).

The samples were analyzed by a laboratory certified to perform organic analyses, using the purge-and-trap (PT) method with a solvent to extract the organic variables and subsequent Gas Chromatograph Mass Spectrometry (GC-MS) analyses. Only the boreholes, in which organic constituents were observed, are listed in **TABLE 7-2** below.

TABLE 7-2

C^T_{obs} **(mg/kg)**

	S1 (17m)	**S1 (18m)**	**S2 (17m)**	**S2 (18m)**	**B8 (18m)**	**B9 (18m)**
Phenol	240	2.4	423	42	112	21
Napthalene	23	2	36	3.6	9	3
Acenapthene	18	1	21	2	11	7
Benzene	62	6	84	7	41	12
M-xylene	162	16	192	17	72	23

7.2.2.1.3 Organic groundwater samples:

A GC-MS scan was run to detect potential organic pollutants. The volatile organics were detected by purge and trap GC-MS based on EPA method 8260. The semi-volatile organics were detected by GC-MS EPA method 8270. The organic groundwater analyses results are presented in **TABLE 7-3**. The MSWQS was used to indicate compliance (JMA, 2003) See Appendix B (included on CD). This is a standard compiled from several international standards, where the most stringent standard was chosen for each variable. South Africa currently does not have local maximum contaminant level standards for organic varibles. Compliance is indicated by values in green, while non-compliance is indicated in red. DL indicates values below the laboratory analysis method detection limit. It can be seen that the S-holes at the source, have the highest contamination values.

TABLE 7-3

Contaminant Grouping		VOC Top					SVOC Middle					
Variable (ppb)		Benzene	m-xylene	Ethylbenzene	Tetrachlorethene	Chloroform	Phenol	Napthalene	Acenapthene	Phenanthrene	Anthracene	Fluoranthene
Boreholes	B1	DL	DL	DL	DL	DL	DL	50	DL	DL	DL	DL
	B2	DL	DL	DL	DL	DL	DL	40	DL	DL	DL	DL
	B3	DL	DL	DL	DL	DL	DL	50	DL	DL	DL	DL
	B4	DL	DL	DL	DL	DL	DL	40	DL	DL	DL	DL
	B5	4	55	8	DL	DL	58	6900	8	7	DL	DL
	B6	5	58	8	DL	DL	40	7000	9	9	DL	DL
	B7	DL	DL	DL	DL	DL	DL	110	DL	DL	DL	DL
	B8	DL	2	2	DL	DL	10	50	3	1	DL	DL
	B9	55	DL	DL	6	23	1400	11000	8	7	6	2
	B10	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL
	B11	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL
	R1	DL	20	7	DL	DL	15	10	1	DL	DL	DL
	R2	DL	DL	DL	DL	DL	DL	8	DL	DL	DL	DL
	S1	80	420	87	32	463	2300	21000	15	16	12	3
	S2	77	320	92	29	589	2100	15000	14	14	10	2
MSWQS (ppb)		3	70	15	5	80	2000	70	5	5	5	1
Contaminant Grouping		VOC Middle					SVOC Bottom					
Variable		Benzene	m-xylene	Ethylbenzene	Tetrachlorethene	Chloroform	Phenol	Napthalene	Acenapthene	Phenanthrene	Anthracene	Fluoranthene
Boreholes	B1	DL	DL	DL	DL	DL	8	DL	DL	DL	DL	DL
	B2	DL	DL	DL	DL	DL	10	DL	DL	DL	DL	DL
	B3	DL	DL	DL	DL	DL	11	DL	DL	DL	DL	DL
	B4	DL	DL	DL	DL	DL	10	DL	DL	DL	DL	DL
	B5	5	21	7	1	29	71	6100	7	6	DL	DL
	B6	12	30	7	3	31	150	3200	6	8	DL	DL
	B7	DL	DL	DL	DL	DL	DL	65	DL	DL	DL	DL
	B8	DL	DL	DL	DL	DL	4	15	2	1	DL	DL
	B9	65	180	50	10	96	950	9900	7	6	5.5	1
	B10	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL
	B11	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL
	R1	DL	21	DL	DL	7	20	DL	1	DL	DL	DL
	R2	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL
	S1	120	710	147	50	700	1900	26000	17.4	16.4	10	7
	S2	39	250	150	30	900	1600	10000	16	16	8	6
MSWQS (ppb)		3	70	15	5	80	2000	70	5	5	5	1

DL = Below Detection Limit

MSWQS = Most Stringent Water Quality Standard: Compliant / Non-compliant

7.2.2.1.4 Parameter determination results for the NAPL sample

The following values were determined (hypothetically) for the parameters - dynamic viscosity, fluid density, contact angle and interfacial tension. These values were determined in a laboratory from the NAPL sample obtained during the drilling of borehole S2. Density measurements were done according to method ASTM D1217-93. Viscosities were determined using a Brookfield Rotational Viscometer by method ASTM D1296. Interfacial tension measurements were done using a Fischer surface tensiometer, according to method ASTM D971. The contact angle was determined using a Camtel CDCA-100 instrument and the Wilhelmy plate method.

Dynamic viscosity (π)	0.015 kg/ms
Fluid density (ρ)	1080 kg/m^3
Contact angle (q)	30 degrees
Interfacial tension (s)	0.01 N/m

7.2.2.2 Analyses

7.2.2.2.1 Analyses and interpretation of soil sample results

Soil characterization programmes typically involve sending discrete soil samples to the laboratory for quantitative analysis of contaminant composition. The presence of NAPL in a soil sample can be evaluated using (Environment Agency, 2003):

$$C_i^T = \frac{C_i}{P_b}(K_d P_b + \theta_w + H'\theta_a) \qquad \text{Equation 7-1}$$

where:

C_i^T	is the concentration of an organic substance at or above that which may be present in a non-aqueous phase (*mg/kg*)
C_i	is the effective solubility of the substance in groundwater *(mg/L)*
P_b	is the dry soil bulk density *(kg/L)*
K_d	is the soil-water partition coefficient *(L/kg)*
θ_w	is the water-filled porosity *(dimensionless)*
H'	is the unitless Henry's Law constant *(dimensionless)*
θ_a	is the air-filled porosity *(dimensionless)*

Equation 7-1 represents the maximum amount of contaminant that can be present in a soil sample in the sorbed, aqueous and vapour phases without a NAPL phase being present. If reported soil concentrations exceed, it can be concluded that free NAPL phase was present in the sample. If the DNAPL is known to

be composed of primarily one component, the mole fraction of that component can be assumed to be one. At sites where a multi-component DNAPL is suspected and a DNAPL sample has not been obtained for component composition analysis, the required mole fractions will not be known. In such cases, this calculation procedure can still be employed, but with a modification (Environment Agency, 2003).

For a multi-component DNAPL of unknown composition, the sum of the mole fractions must equal one. DNAPL will therefore be present in a soil sample if the following condition is met:

$$\sum_{i=l}^{n} \frac{C^{T}_{obs}}{C^{T}_{S}} \geq 1$$

Equation 7-2

where:

C^{T}_{obs}	is the reported concentration of component *i*
C^{T}_{S}	is the single component soil concentration of component *i*
n	is the total number of components observed in the soil sample

In the tables below, the sum of the reported concentration values divided by the single component soil concentrations, have been calculated. The following information has been obtained in the following ways:

C^{T}_{i}	values have been obtained by performing GC-MS analyses on the soil samples (*mg/kg*)
C_i	the effective solubilities of the substances in groundwater *(mg/L)* – have been obtained from textbooks
P_b	is the dry soil bulk density *(kg/L)* and has been determined by a soil laboratory
K_d	is the soil-water partition coefficient *(L/kg)* has been determined by the equation $\mathrm{Kd} = \mathrm{koc} \times \mathrm{foc}$ (Karickhoff, 1981)
Koc	is the octanol-water partition coefficient that is a textbook value that has been laboratory determined
foc	is the fraction of organic carbon, determined by a soil analyses laboratory. This was determined indirectly by determining the total carbon, then ashing the sample and determining the inorganic carbon from the ash. The organic carbon content is derived from subtracting the inorganic carbon from the total carbon. The foc is the ratio of the TOC to the total carbon.
θ_w	is the water-filled porosity *(dimensionless)* and has been determined by a soil analyses laboratory
H'	is the unitless Henry's Law constant (*dimensionless*) and has been obtained from textbooks
θ_a	is the air-filled porosity *(dimensionless)* and has been determined by a soil analyses laboratory

The following are constants in the equations used to determine the data presented in the tables below:

P_b	1.99 *kg/L*
foc	0.001
θ_w	0.2 (20%)

θ_a 0.1 (10%)

Borehole S1 (17m):

TABLE 7-4

Compound	C^T_{obs} (mg/kg)	Koc (L/kg)*	Maximum Solubility (mg/L)*	Henry's Law Constant (dimensionless)*	C^T_S (mg/kg)	$\frac{C^{T_{obs}}}{C^{T_S}}$
Phenol	**240**	10041	82800	0.0000136	831395	0.000289
Napthalene	**23**	1191	32	0.018	38.3138	0.600306
Acenapthene	**18**	7832	3.47	0.00744	27.377784	0.657467
Benzene	**62**	87.78	1780	0.227	156.4711	0.396239
M-xylene	**162**	775	180	0.294	139.7294	1.159384
					SUM =	2.813685

- *See Appendix A, Data Set 1and 2, Chapter 4*

The sum of $\frac{C^{T_{obs}}}{C^{T_S}}$ has been determined for boreholes S1 (18m), S2 (17 and 18m), B8 (18m) and B9 (18m).

The results were as follows:

S1 (18m)	0.2415
S2 (17m)	3.6180
S2 (18m)	0.3335
B8 (18m)	1.4143
B9 (18m)	0.5753

In all of the above boreholes, except borehole S1 (18m), S2 (18m) and B9 (18m) the following condition is met: $\sum_{i=l}^{n} \frac{C^T_{obs}}{C^T_S} \geq 1$

Since borehole S1 (18m), S2 (18m) and B9 (18m) is less than 1, it cannot be concluded that NAPL was present in that sample. It can be concluded that NAPL phase was likely in all the other samples.

7.2.2.2.2 Analyses and interpretation of organic groundwater samples

The contaminant concentrations in the groundwater have been analyzed to determine the possibility of the presence of a NAPL source in the vicinity. Experience has shown that DNAPL may be present up–gradient of a monitoring well displaying sampled groundwater concentrations in excess of one percent of the effective solubility of the component of interest (Environment Agency, 2003).

Calculating the one percent effective solubility requires a priori knowledge of the DNAPL composition such that mole fractions can be established. If the DNAPL is thought to be composed of primarily one component, the mole fraction of that component can be approximated to be one. If the DNAPL is thought to be composed of several components, however, a modified approach will be required in cases where a DNAPL composition analysis is not available. For a multi-component DNAPL dissolving into groundwater, the equilibrium aqueous phase concentration can be represented using Raoult's law. (See equation 7-4 below).

Because groundwater concentrations are typically obtained from monitoring well samples, a certain degree of dilution will occur due to borehole dilution, hydrodynamic dispersion, non-optimal well placement and degradation. In this analysis, the degree of dilution due to these three processes will be represented by the parameter *a*, such that:

$$a = \frac{C_i^{obs}}{C_i} \qquad \textit{Equation 7-3}$$

where:

C_i^{obs} is the concentration observed in the monitoring well

C_i is the effective solubility given by equation 7-4

$$C_i = x_i S_i \qquad \textit{Equation 7-4}$$

Ci is the effective solubility of component *i*

x_i is the mole fraction of component *i* in the NAPL

Si is the single component solubility of component *i*

For a multi-component NAPL, the sum of the mole fractions must equal one:

$$\frac{C_i}{S_i} = 1 \qquad \textit{Equation 7-5}$$

Combining equations 7-3 and 7-5, gives:

$$\frac{C_i^{obs}}{S_i} = a \qquad \textit{Equation 7-6}$$

If the one percent 'rule-of-thumb' is adopted, it follows that DNAPL may be present upstream of a monitoring well if ***a*** **>0.01**. This assumes that the degree of borehole dilution, dispersion and degradation is identical for each component of interest. This is likely to be the case for borehole dilution and dispersion, but may not be the case for degradation. For monitoring wells in close proximity to DNAPL, however, the amount of degradation may be minimal such that the error introduced by varying amounts of degradation will be negligible. The values obtained at different sampling depths per one contaminant, have been totaled per borehole.

In **TABLE 7-5** below, an example is given of the calculation of "*a*" for borehole B8.

TABLE 7-5			
Compound	**Concentration in monitoring well (Ci) (mg/L)**	**Single component solubility (Si) (mg/L)***	$\frac{Ci}{Si}$
Naphthalene	0.065	32	0.002031
Benzene	0	1780	0
m,p-Xylene	0.002	180	1.11E-05
Ethylbenzene	0.002	150	1.33E-05
Tetrachloroethene	0	150	0
Chloroform	0	8000	0
Phenol	0.014	82800	1.69E-07
Acenaphthene	0.005	3.47	0.001441
Phenanthrene	0.002	1.18	0.001695
Anthracene	0	0.073	0
Fluoranthene	0	0.265	0
$a = \sum \frac{C_i^{obs}}{S_i}$			0.005192

* *See Appendix B1 and B2, Chapter 3*

In **TABLE 7-6** the "a" values are given, as calculated for each of the boreholes in which organic contamination was observed.

TABLE 7-6	
Borehole	**"a"**
B1	0.00156
B2	0.00125
B3	0.00156
B4	0.00125
B5	0.42213
B6	0.33810
B7	0.00547
B8	0.00519
B9	0.83887
R1	0.00117
R2	0.00025
S1	1.85334
S2	1.09755

From **TABLE 7-6** it can be seen that boreholes B5, B6, B9, S1 and S2 have "a" values are above 0.01, which indicates the presence of NAPL upstream or in the vicinity of the borehole. Boreholes S1 and S2 have the highest "a" values and indicate the source boreholes.

Identification of the type of organic contaminant:

The following method has been developed by Powers, Villaume and Ripp (1997) and attempt to identify the type of parent product of the dissolved phase hydrocarbons. They made 'star' plots with four axis of parent products – one axis for benzene (B), one for toluene (T), one for ethylbenzene (EB) plus xylenes (X) and one for naphthalene (N). The data is normalized by summing the total of all the components and dividing the individual components by the total.

The analyzed groundwater components were plotted in a similar way to derive a star plot. The values obtained from all the groundwater analyses on the site were totaled for each constituent in order to obtain an average. The representative concentrations for each component (micrograms per liter) is shown below:

Constituent	*Concentration (ppb)*	*Normalized value*
Naphthalene	116538	0.9740
Benzene	462	0.0039
m-xylene + Ethylbenzene	2652	0.0221
Sum	119652	1

If the above data is plotted, the resultant diagram is very similar to the diagram for creosote plotted by Powers *et al* (1997) (see **Figure 7-8**), and it can be assumed that the water at the site represent a creosote type of NAPL contamination. The similar was done for boreholes S1 and S2, with similar results. Boreholes far from the source (see R2) where selective degradation and sorption already occurred with the dissolved NAPL will not be representative, since the representative variables will not be present in the correct relative concentrations. Data manipulation can be seen in **APPENDIX C**, where it can also be seen that most of the holes close to the source represent creosote type NAPL.

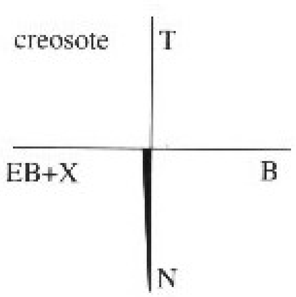


Figure 7-8 (Creosote identification diagram)

7.2.2.3 Movement of organic contaminants in different zones of the aquifer

Napthalene has been sampled for SVOC middle and bottom, with an extra sample taken at a depth between these two sampling depths, and a comparison of these values can be seen in **FIGURE 7-9**. This has been done in order to compare the movement of naphthalene in the horizontal and transverse directions. Benzene has been sampled in a similar way and can be seen in **FIGURE 7-9**. The red indicates non-compliance in terms of the MSWQS.

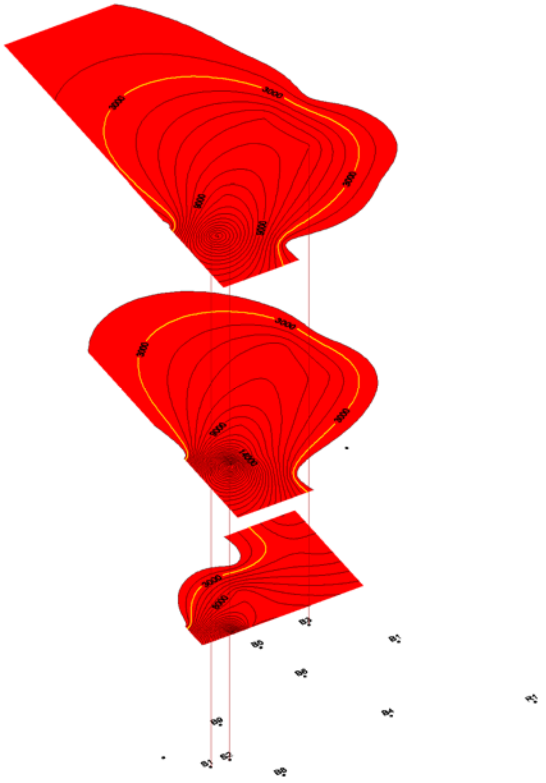


Figure 7-9 (Naphthalene depth comparison)

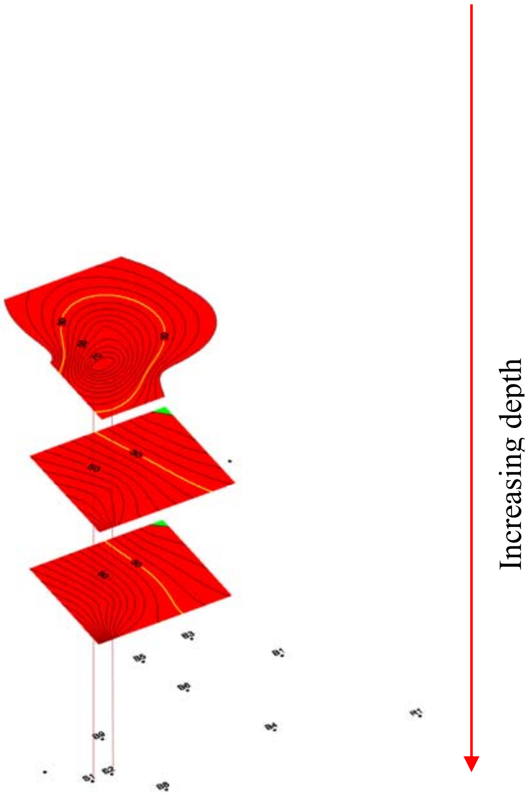


Figure 7-10 (Benzene depth comparison)

Comparing the above contours for the naphthalene (**FIGURE 7-9**), the following can be seen:

- The naphthalene developed the dissolved phase plume most extensively in the top of the aquifer.
- The naphthalene for the bottom of the aquifer shows the least extensive dissolved phase plume.

From the above the following can be concluded: PAH's (like naphthalene) sorb strongly to soil and are very hydrophobic (Environment Agency, 2003). This can be seen due to the fact that the naphthalene has not migrated deep into the aquifer and is still associated with the shallower soils.

In order to show that benzene moves more readily than naphthalene, it has been plotted in a similar manner. It can be seen from **FIGURE 7-10** that benzene moved deeper into the aquifer than naphthalene, which can mostly be seen in the top zone of the aquifer, where it has sorbed onto particles. In both the naphthalene and benzene figures, the yellow line represents a constant value at each depth. Benzene is an aromatic hydrocarbon that partitions more readily into the vapour phase and would thus partition more readily into the groundwater (and will spread easier) than the naphthalene, which is a non-aromatic hydrocarbon (Fetter, 1999). This can also be seen when comparing Kow values of benzene (87.78 mL/g - moderate adsorption capacity) versus naphthalene (1203 mL/g - strong adsorption capacity). Factors such as density and viscosity were not taken into account for this study but would play a large role in NAPL movement.

7.2.2.4 Calculation of fracture apertures, entry pressures and NAPL pool heights

Data from the 15 drilled boreholes have been used to calculate the entry pressures for the horizontal fractures encountered on site.

The formula for transmissivity has been used to calculate fracture apertures in the following way (the cubic law):

$T = \rho g / 12\pi \, (2b)^3$ (Snow,1969) *Equation 7-7*

Thus the fracture aperture can be calculated by re-writing the equation as:

$b = 0.5 \times (T12\pi/\rho g)^{1/3}$ *Equation 7-8*

where:
T = transmissivity (m^2/s)
ρ = fluid density (kg/m^3)
g = acceleration due to gravity (m/s^2)
π = dynamic viscosity (kg/ms)
b = fracture aperture (m) – the same as 'e' in Equation 7-9.

For all boreholes drilled on a site, the total yield of each borehole can be calculated to fractions of yields by dividing the specific yield of a fracture zone by the total yield of the borehole. If all the factors are added together, it gives one, the total yield of the borehole. The K-value for each fracture is calculated by multiplying each factor (determined above) by the total K-value derived from the slug test. Dividing this by 86400 seconds (24 hours) converts the K-value from m/d to m/s. After determining the K-value for each fracture, the aperture is calculated using $b = 0.5 \times (T12\pi/\rho g)^{1/3}$, where:

$T = Kd$

K	is the determined permeability for each fracture (m/s)
d	is the *flow zone* in meters (the top water strike subtracted from the bottom water strike)
π	is 0.001 kg/ms (laboratory determined)

ρ is 1000 kg/m^3 (laboratory determined)
g is 9.8 m/s^2

The following limitations exist for the above technique:
When performing a slug test in a fractured rock environment, the K-value reflects only the effect of the fractures and not the rock matrix (Lerner and Steele, 2001). In addition, the K-value usually reflects the effect of the largest aperture, which is the flowpath of least resistance (Vermeulen and Van Tonder, 2004). For the above method to yield and average correct answer for all fractures considered, it will be best is all the fractures were equal and spaced equidistant (in this way they will simulate a homogenous porous flow model). If fractures were spaced far apart, the fracture closest to the slug will be influenced the most. This means that the following conditions must be met for application of the above method:

- The fractures must all be of relatively the same size.
- The fractures must be spaced closely together and preferably equidistant and parallel.

The aperture can also be inferred from core drilling recoveries, but only solid rock is retrieved from core drillings while fractures are not recovered, which makes estimation of the fracture aperture problematic. A sonic log would produce a digital log of fracture positions, orientation and aperture, and in the absence of sonic, a down-the-hole video's can be used to overcome this problem. Where the fracture intersects the whole borehole, the direction of dip of the fracture (and thus the direction of possible NAPL flow can be determined). However, only the surface of the fracture wall can be seen with a down-the-hole camera, so the deeper fracture aperture can not be measured directly with a camera.

The above method was tested on borehole UO5 on the campus test site of Institute for Groundwater Studies (IGS). The slug test data was applied on a flow zone of 20m. The K-value obtained was 17 m/d (for total length of open well screen) and was determined with the Bouwer and Rice method as presented in the Flow Characteristic (FC) program developed by the IGS. This equals a K of 0.000197 m/s.

Only one factor is applicable since only one fracture was encountered, thus the K-value for one fracture = 0.000197 m/s. The flow zone is estimated to be 1m (water strike information). The hydraulic aperture has been calculated using the data above and is equal to 0.000313 m. The aperture, calculated with a numerical model for a K of 17 m/d, is 0.0003 m. Applying a K-value of 600 m/d, an aperture of 0.001 m is obtained, which is the same for the campus aquifer.

The campus test-site data, however, could not test the theory in full, because only one fracture was encountered. It should be tested against an aquifer containing at least two major fractures / fracture zones, of which the water strikes would be relatively close to each other (such that the slug test would influence both fractures) and the top and bottom water strikes for each should be the same (such that the flow zones would be roughly the same and thus the estimates of aperture correct). The apertures should be calculated and the boreholes and then logged with down-the-hole video in order to determine the visual apertures. There still is the question regarding visual aperture and the hydraulic aperture, in whether the visual measurements are misleading or not, and whether the hydraulic aperture calculations are an under- or over-estimate of the true (effective) aperture.

Slug tests were performed on all 15 boreholes and a general K-value for each borehole was obtained. Since the boreholes are drilled in hard rock formation, the contributing factor towards the K-values was deemed to be the fractures and not the rock matrix. The 15 boreholes encountered 29 fractures (water strike zones) in total and some of these were used to determine apertures and entry pressures, in other cases fracture apertures were measured with down-the-hole video camera, and the entry pressures determined from those apertures (see **TABLE 7-8**).

An example of the aperture calculations is given in **TABLE 7-7** below:

TABLE 7-7				
Borehole	**Factor 1**	**Factor 2**	**K1 (m/s)**	**K2 (m/s)**
B7	0.5	0.5	2.35E-06	2.35E-06
	Flow zone 1	**Flow zone 2**	**Aperture 1 (m)**	**Aperture 2 (m)**
	1	1	7.17458E-05	7.17E-05

Once the fracture aperture has been determined, the entry pressure for NAPL can be determined, with the following equation:

Pe = (2.s.cos(q))/e (Pankow and Cherry, 1996) *Equation 7-9*

Where

Pe = Entry Pressure (Pa)
s = Interfacial tension (N/m) = 0.01 N/m (laboratory determined)
q = contact angle (degrees) = 30 degrees (laboratory determined)
e = fracture aperture (m)

See **TABLE 7-8** for the calculated entry pressures. Assuming that the range of fractures and associated apertures in the vertical direction will be roughly the same as in the horizontal direction for a fracture network in a dolerite sill, a range of possible critical pool heights that may exist in the fracture network has been determined.

In order for a NAPL to enter a fracture, the capillary pressure at the entrance of the fracture must exceed the entry pressure of the fracture (Pe). The capillary pressure may be expressed as height of pooled NAPL (assuming static equilibrium).

The height of the vertical pool is given by:

Hd = $\frac{2\sigma}{\Delta\rho g e}$ (Kueper and McWorther, 1991) *Equation 7-10*

Hd = Height of pooled NAPL
σ = interfacial tension between NAPL and water (N/m) = 0.01 N/m
$\Delta\rho$ = density difference between NAPL and water (kg/m3) = 1080 kg/m3 – 1000 kg/m3 = 80 kg/m3
g = gravity (m/s2) = 9.8 m/s2

Thus the ranges of pool heights vary between 5.187 m for the smallest aperture in the range (8.18E-6 m) and 0.211 m for the largest aperture (0.000201 m). See **APPENDIX D** for the calculations of values presented in **TABLE 7-8**.

TABLE 7-8

Bore-Hole	**Flow zone Bottom w/s -Top w/s**	**Comment**	**Method Applied (Y/N)**	**Aperture (m)**	**Entry Pressure (Pa)**
B1	2	Single fracture zone	Y	4.44E-05	390.218
B2	2	Relatively equidistant, equal size apertures	Y	7.18E-05	241.2931
	2			7.18E-05	241.2931
	1.8			6.93E-05	249.9043
B3	1	Single fracture zone	Y	2.01E-04	86.28437
B4	0.5	Relatively equidistant, equal size apertures	Y	4.27E-05	405.5635
	0.6			4.54E-05	381.6731
B5	1	Fractures not equidistant; different sizes	N	4.71E-05	367.9012
	1			8.55E-05	202.5848
B6	1	Fractures not equidistant; different sizes	N	1.52E-05	1137.515
	1			2.27E-05	761.7958
	0.5			2.27E-05	761.7958
	3			5.2E-05	333.0207
B7	1	Relatively equidistant, equal size apertures	Y	7.17E-05	241.4151
	1			7.17E-05	241.4151
B8	1	Fractures not equidistant; different sizes	N	2.22E-05	779.8952
	2			3.52E-05	491.5303
B9	1	Fractures not equidistant; different sizes	N	3.71E-05	467.1494
	3			1.56E-04	110.9329
	2			7.19E-05	240.7886

TABLE 7-8					
Bore-Hole	**Flow zone Bottom w/s-Top w/s**	**Comment**	**Method Applied (Y/N)**	**Aperture (m)**	**Entry Pressure (Pa)**
B11	2.5	Fractures not equidistant; different sizes	N	6.59E-05	262.6482
	1			6.12E-05	282.9081
	1			1.40E-04	123.6739
	1			1.38E-04	125.4391
B12	1	Single fracture zone	Y	4.31E-05	401.6899
B13	2	Single fracture zone	Y	4.97E-05	348.3393
B14	2	Single fracture zone	Y	9.75E-05	177.6396
B15	2	Single fracture zone	Y	1.23E-04	140.2962

The apertures have been plotted against the entry pressures and the results are shown in **FIGURE 7-11**

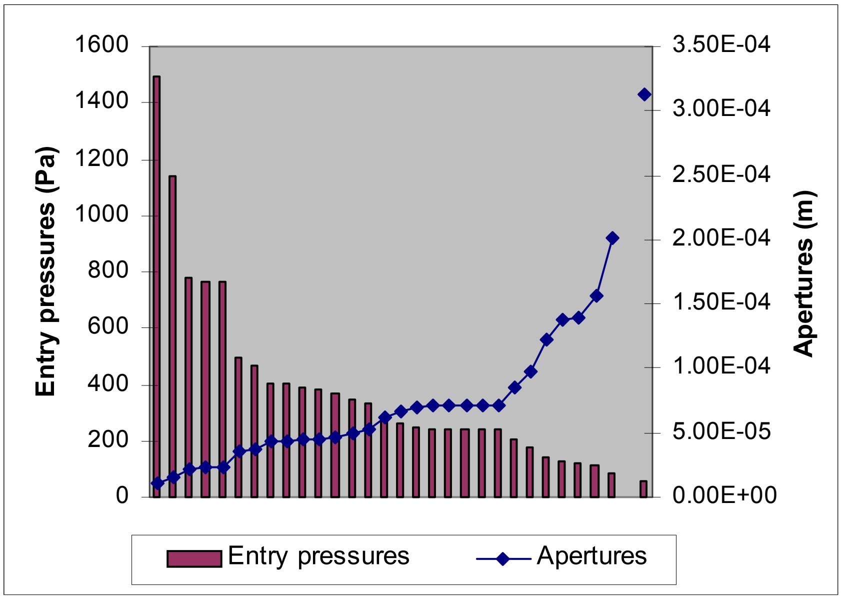


Figure 7-11 (Graph of apertures against entry pressures)

From the above figure it can be seen that the larger the aperture, the smaller the entry pressure needed to enter the fracture. The vertical NAPL pool height and entry pressures are proportional and a larger aperture is related to a smaller pool height. See **FIGURE 7-12.** These pool heights are inferred possible heights in order to obtain a range of pool heights, which may exist above vertical fractures in the fracture network. The results are considered as fairly valid given the construction of boreholes – the slotted casing was inserted along the largest length of the borehole, thus hydraulic reactions in the borehole should be fairly close to natural circumstances (i.e. if no casing were inserted over the depths of measurement).

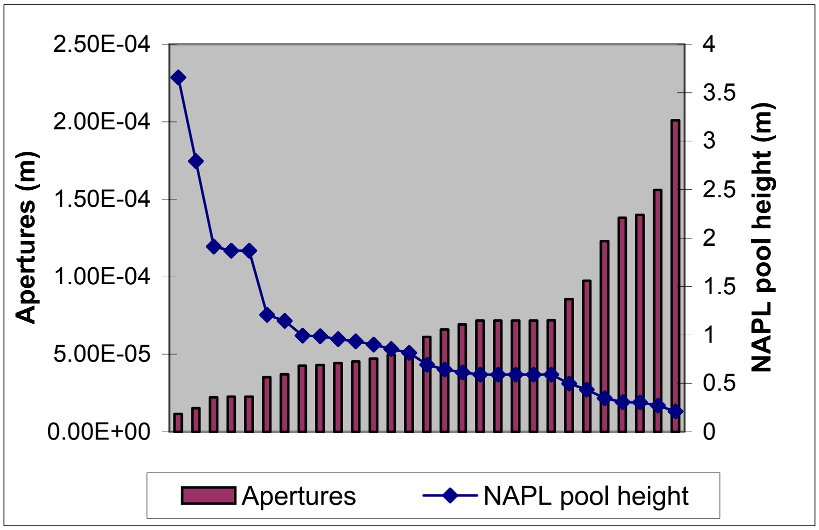


Figure 7-12 (Graph of apertures against pool heights)

7.2.2.5 Final conceptual model

The information obtained during the site characterization, has been used to draw a final conceptual model of the site, which is shown in **FIGURE 7-13.**

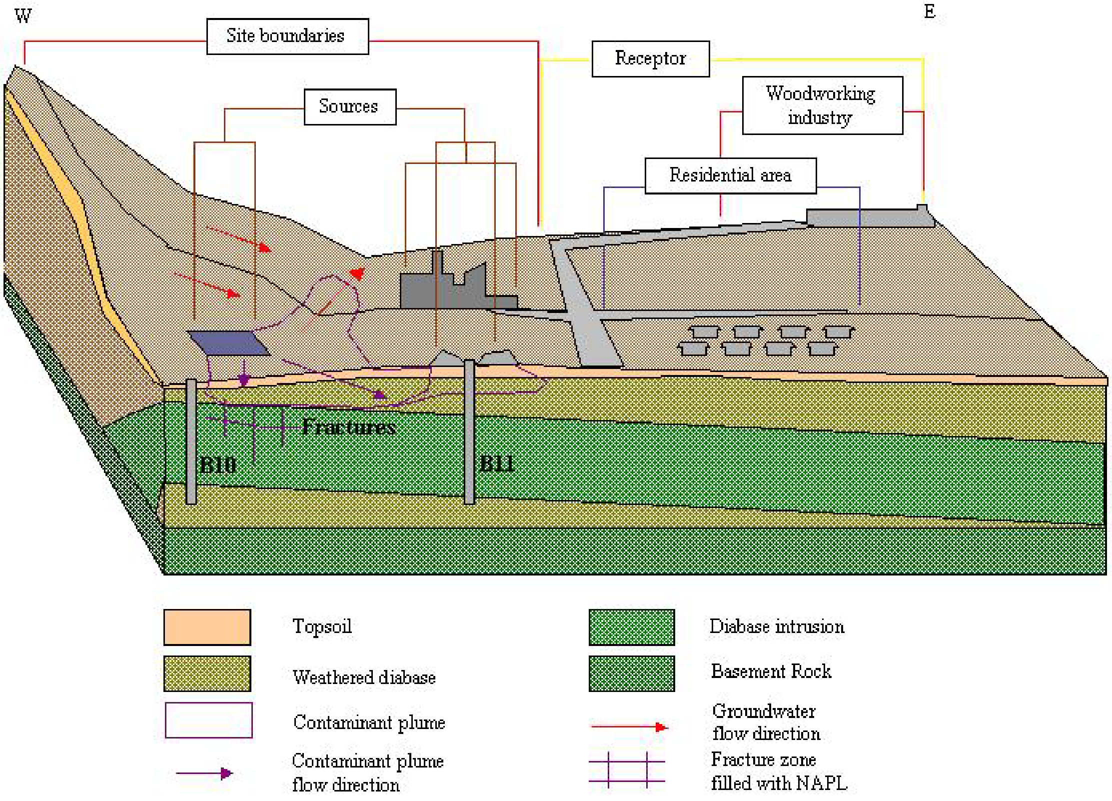


Figure 7-13 (Final conceptual model)

The following comments are relevant to the final conceptual site model:

- Boreholes B10 and B11 have only been drilled during the site characterization phase and logging of the diabase interceptions in the boreholes have shown that the diabase intrusion dips towards the southeast. This has been confirmed with down-the-hole video footage.
- During groundwater analyses and subsequent contouring of the chemical data, it has been observed that groundwater is polluted in the eastern direction of the site, apart from the groundwater pollution observed towards the northeast (in the direction of groundwater flow). This can be explained at the hand of the diabase intrusion of which the fractures serve as a preferential pathway for mostly the organic pollutants, and in a lesser degree for the inorganic pollutants.
- The minimum entry pressure needed for the DNAPL to enter the top aquifer fractures is 82 Pa (0.000211 m aperture), and the maximum needed to enter the bottom aquifer fractures is 2016 Pa (8.59E-06 m aperture). The minimum pool height required for entry is 0.201 m (200 cm), which is not foreseen to exist on site since such a large amount of NAPL has not been dumped. Given this, and the fact that fracture apertures decrease with depth (Schechter, 2002), it is not foreseen that the DNAPL will enter deeper than it currently entered the aquifer zone. From laboratory test results of viscosities at different temperatures, it has also been determined that the NAPL will not be very mobile at depth in the aquifer. Lateral movement of the DNAPL on top of the diabase intrusion towards the east, is however, not excluded, and diffusion into the dissolved phase still poses a large problem. Degradation may lower the rate of dissolution into the groundwater.

7.3 IMPACT DESCRIPTION

The groundwater impact for the organic chemistry is described at the hand of compliance contour maps. The contour maps have been drawn up as a first step towards describing the impacts at the site and the influence on the receptor. The contour maps will be used to draw up a boundary compliance table, which will highlight pollutants of concern. This information will also be used in the aspect and impact register.

7.3.1 Organic impact description

Contour maps of the organic variables totaled:

Contour maps of the (hypothetical) organic results have been drawn up for the total organic pollution values and are given in **FIGURES 7-14 - 7-17**. Only boreholes in which organic pollution were identified, were plotted, but it should be noted that liquid NAPL that does not show in the other boreholes, might have migrated further down or to other areas in the aquifer. A borehole camera was sent down the holes and no large fractures were identified in the clean boreholes, thus lowering the chance of NAPL that migrated downward. Further investigation could be launched by drilling very deep telescoped boreholes but the chance of picking up this dispersed NAPL is unlikely. It should be kept in mind for remediation that NAPL might exist in other areas of the aquifer and that the remediation effort must be expanded beyond the identified NAPL zone.

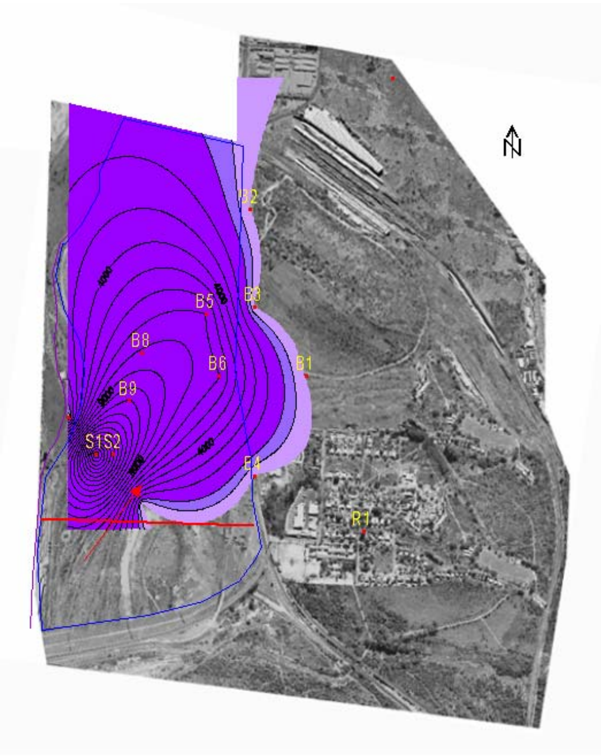


Figure 7-14: VOC top total

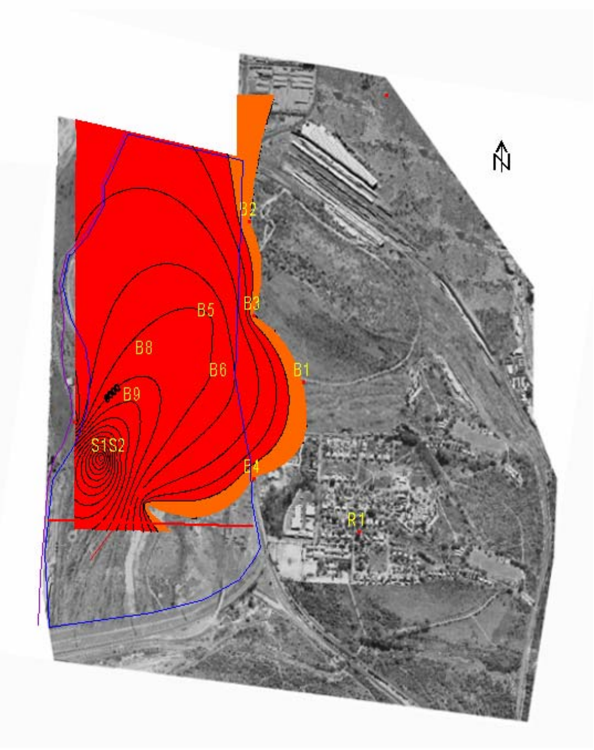


Figure 7-15: VOC middle total

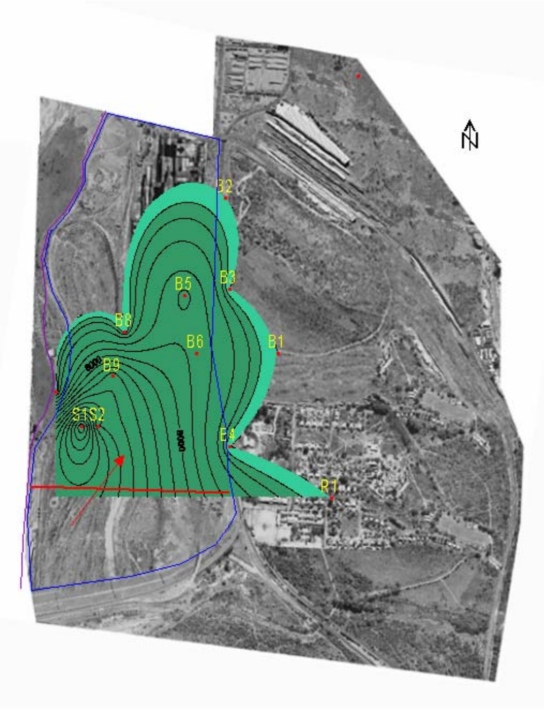


Figure 7-16: SVOC middle total

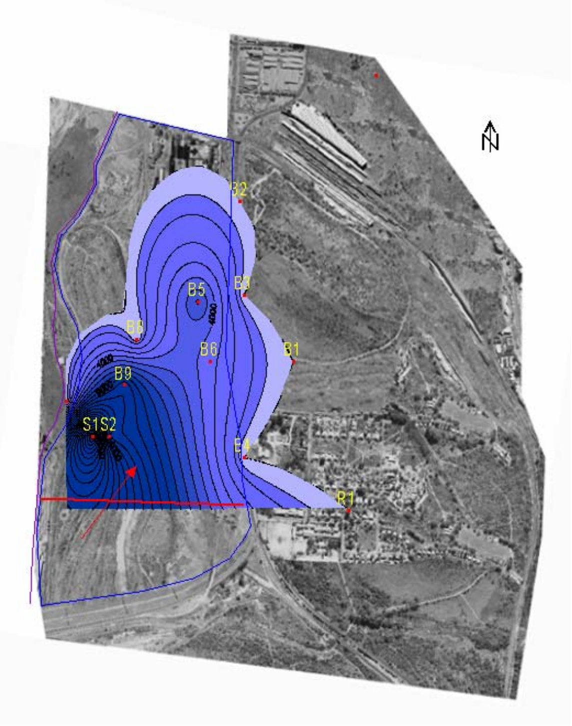
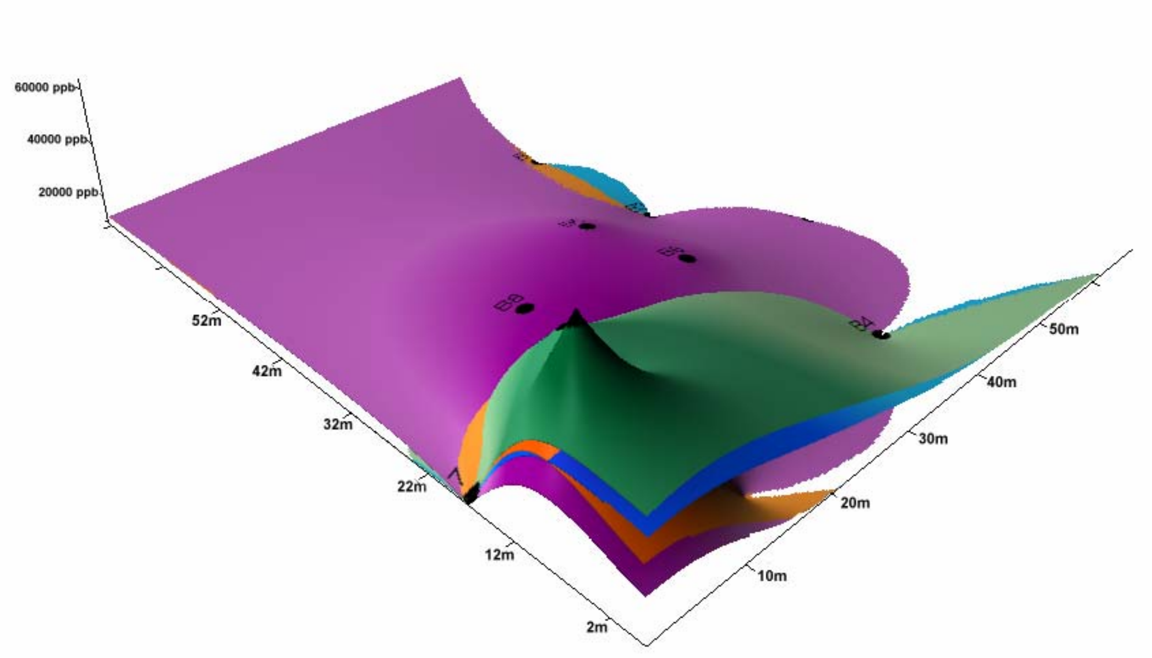


Figure 7-17: SVOC bottom total

From the figures it can be seen that the VOC's all react the same and follows the direction of groundwater flow movement. The dolerite dyke, however, influences the SVOC's flow path. It can be seen that the dyke acts as a preferential flow zone and that SVOC's move towards the east as well as towards the northeast (the groundwater flow direction).

In **FIGURE 7-18** below, the VOC and SVOC totals have been overlayed and are shown as a three dimensional image. The colours represent the same colours as shown in the figures above, so it can be seen that the highest concentration of contaminants is represented by the total SVOCs for the middle of the aquifer. The spread of contaminants are fairly the same for all the depths of samples taken. Hypothetical units have been assigned to represent the size of the pollution plume.



Colour code	Variable	Colour code	Variable
🟪	*VOC top total*	🟩	*SVOC middle total*
🟥	*VOC middle total*	🟦	*SVOC bottom total*

Figure 7-18

Contour maps specific organic variables:

The specific organic variables measured for all depths have been totalled for each borehole to represent the worst case scenario for impact assessment and are shown in **FIGURES 7-19** to **7-29**. Hypothetical units have again been assigned to represent the size of the organic variable pollution plumes.

⬜	Aerial photograph
🟩	Most Stringent Water Quality Standard: Compliance
🟥	Most Stringent Water Quality Standard: Non-Compliance
―	Site Layout

Legend

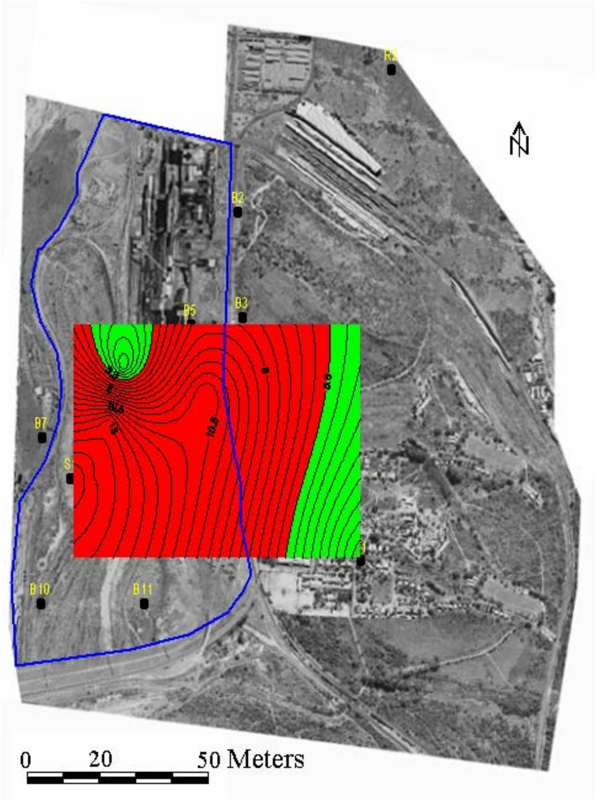
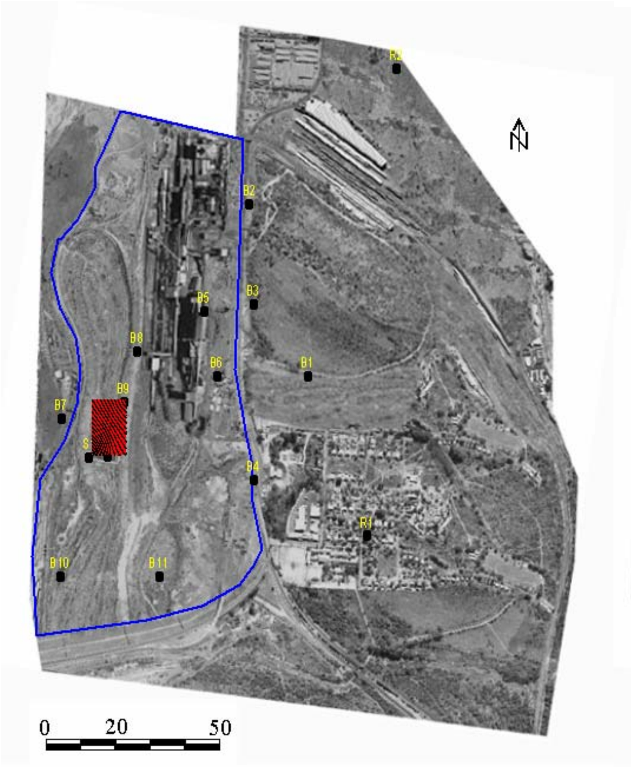


Figure 7-19: Acenapthene



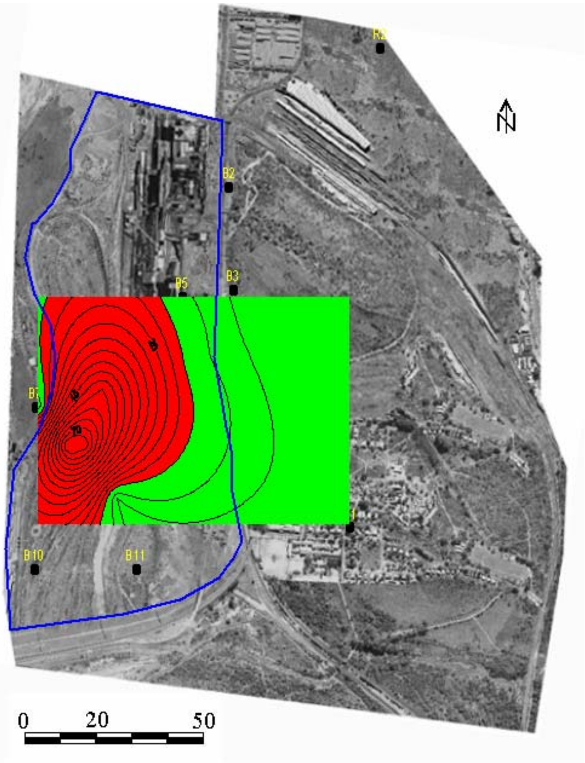


Figure 7-20: Anthracene

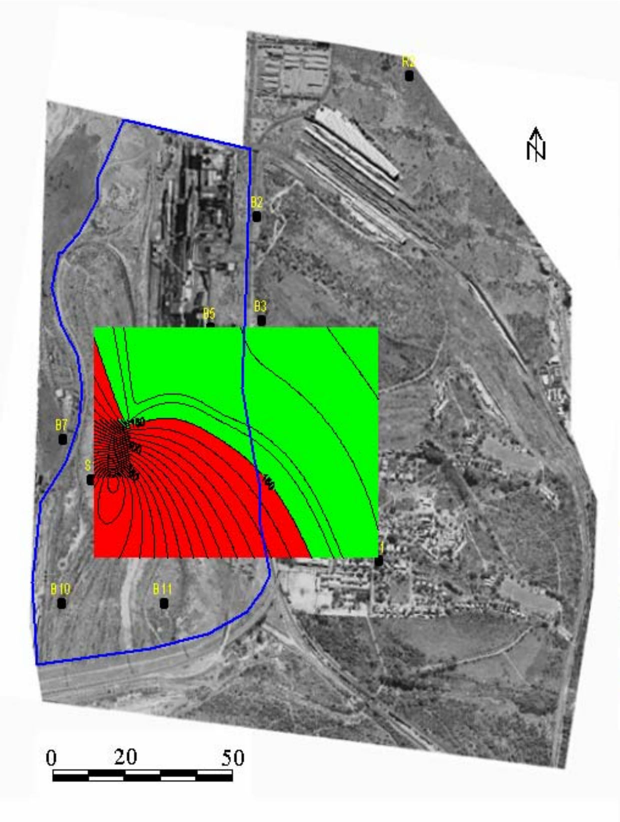


Figure 7-21: Benzene

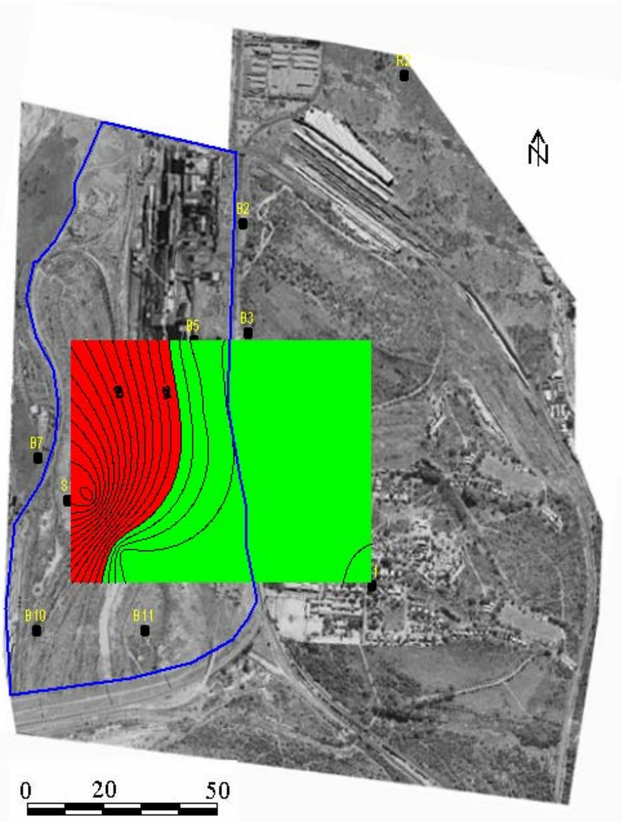


Figure 7-22: Chloroform

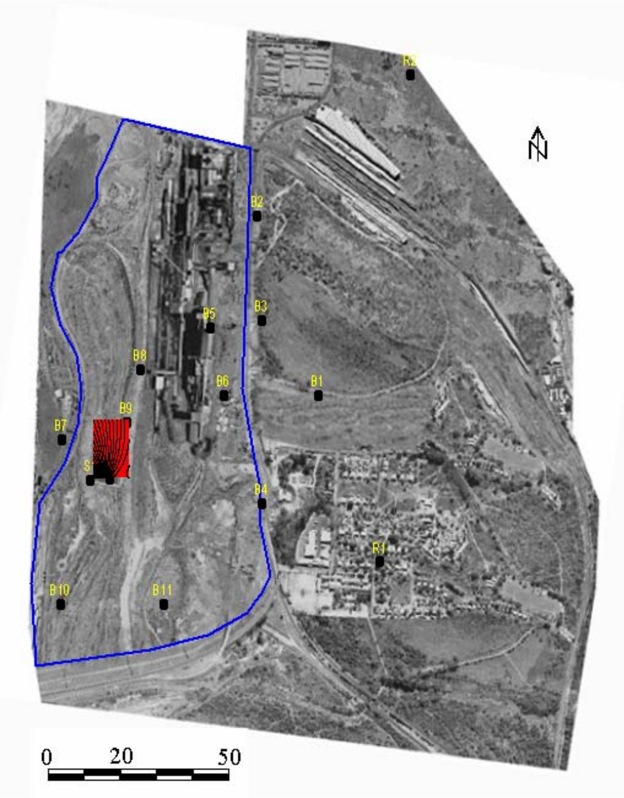


Figure 7-23: Ethylbenzene

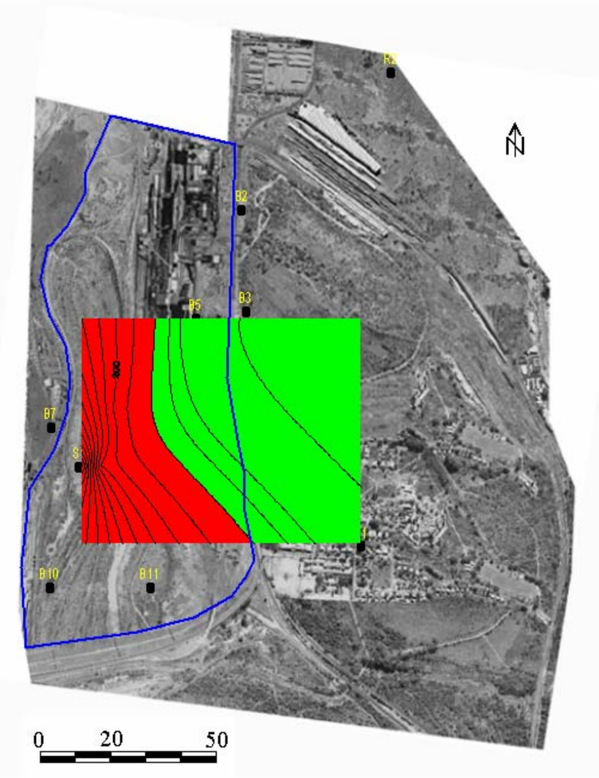
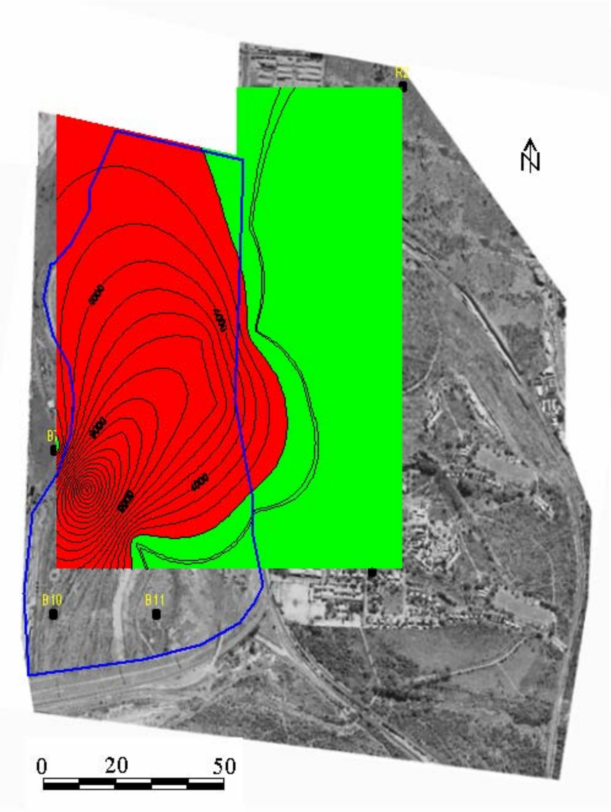


Figure 7-24: Fluoranthene

Figure 7-25: m-xylene



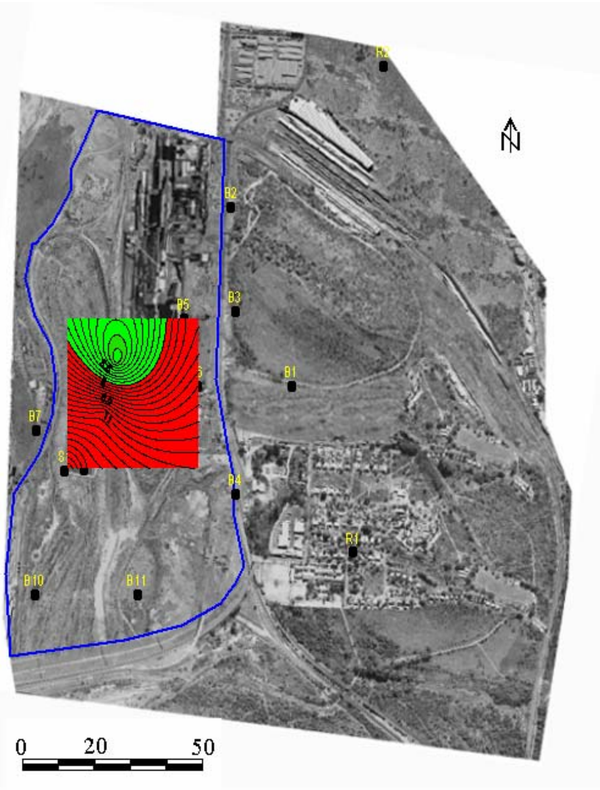


Figure 7-26: Naphthalene

Figure 7-27: Phenanthrene

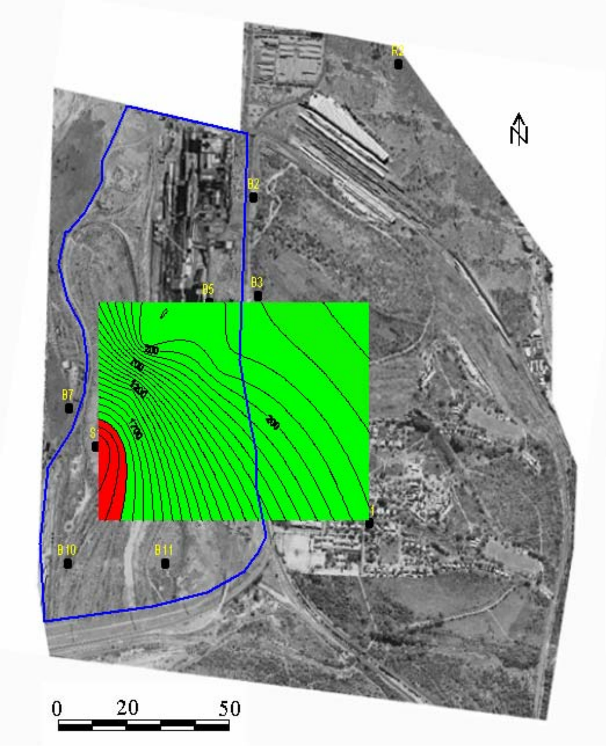


Figure 7-28: Phenol

Figure 7-29: Tetrachlorethene

From the previous figures the following conclusions can be drawn:

- Variables showing non-compliance in terms of the site perimeter are acenapthene, chloroform, m-xylene and naphthalene.
- The constituents that moved the furthest are acenapthene and naphthalene.

The impact assessment follows from the site characterization. **TABLE 7-9** assigns impact ratings to each inorganic variable, which will be used in the impact assessment (section 7.3.3). The qualifying criteria is the following:

Impact rating	**Qualifying criteria**
1	Impact located around the source(s) – low impact
2	Impact covering part of the investigated site but does not extend beyond the site boundaries – medium impact
3	Impact extends beyond the site boundary – high impact

TABLE 7-9 reflects the local impact description, which will be applied in Section 3.4.

TABLE 7-9

Variable	**Impact rating**
Acenaphthene	3
Anthracene	1
Benzene	2
Chloroform	3
Ethylbenzene	2
Fluoranthene	1
M-xylene	3
Naphthalene	3
Phenanthrene	2
Phenol	1
Tetrachlorethene	2

7.3.2 Impact and aspect register

In the aspect and impact register, the aspects that cause impacts are described, and the severity of the impact is rated as well. In order to understand all the possible impactors (sources), the processes and plants on the site, are described below. This will be used to describe the aspect map as well as the impact and aspect register. This information has been obtained from the steel industry itself, via personal communication and internal industry reports. It is very important for industry to keep records of all their plant processes and waste management for site investigations.

Industry processes and plants:

The processes on site are described for the various plants occurring in the plant area of the industry.

Coke Plant - Coal is used at one location, namely the coke plant. The coke plant was needed to produce high temperatures for the melting and rolling of steel. The coke plant consists of five coal ovens, in which pulverized coal is carbonized at temperatures of 1000°C, which drives off most of the volatile gasses. Metallurgical coke remains, which is sent to a dry cooling plant. Various by-products are produced (e.g. naptha, creosote, anthracene oil, tar and pitch).

Blast Furnace Plant - The coke is conveyed to blast furnaces, where together with fluxing material (dolomite) and iron ore, it is fed into different sections of the blast furnace plant. The process in operation is to separate the oxides from the iron in order to produce pig iron. Molten pig iron (the immediate product of smelting iron ore with coke and limestone in a blast furnace, also called raw iron) and molten slag are obtained from the blast furnace plant.

Steel Melting Plant - The molten steel is moved the steel melting plant where it is refined cast into ingots. The slag is cooled, crushed and sold as road metal.

Rolling Mills Plant - The cooled ingots are stripped from the molds and brought to a uniform temperature, after which it is rolled into steel sheets, for selling purposes.

The aspect map:

Before making a list of aspects and impacts, an aspect map was compiled in order to delineate all the possible impact sources, as well as the receptors. This can be seen in **FIGURE 7-30.**

The source and receptor areas have been delineated into four business units (BU), which are:

- The site itself
- The residential area
- The open veld area
- The woodworking industry

The NAPL dump site and evaporation pond, as well as the plant area and the raw material storage area sort under the site and are not specified as business units. These represent contamination sources.

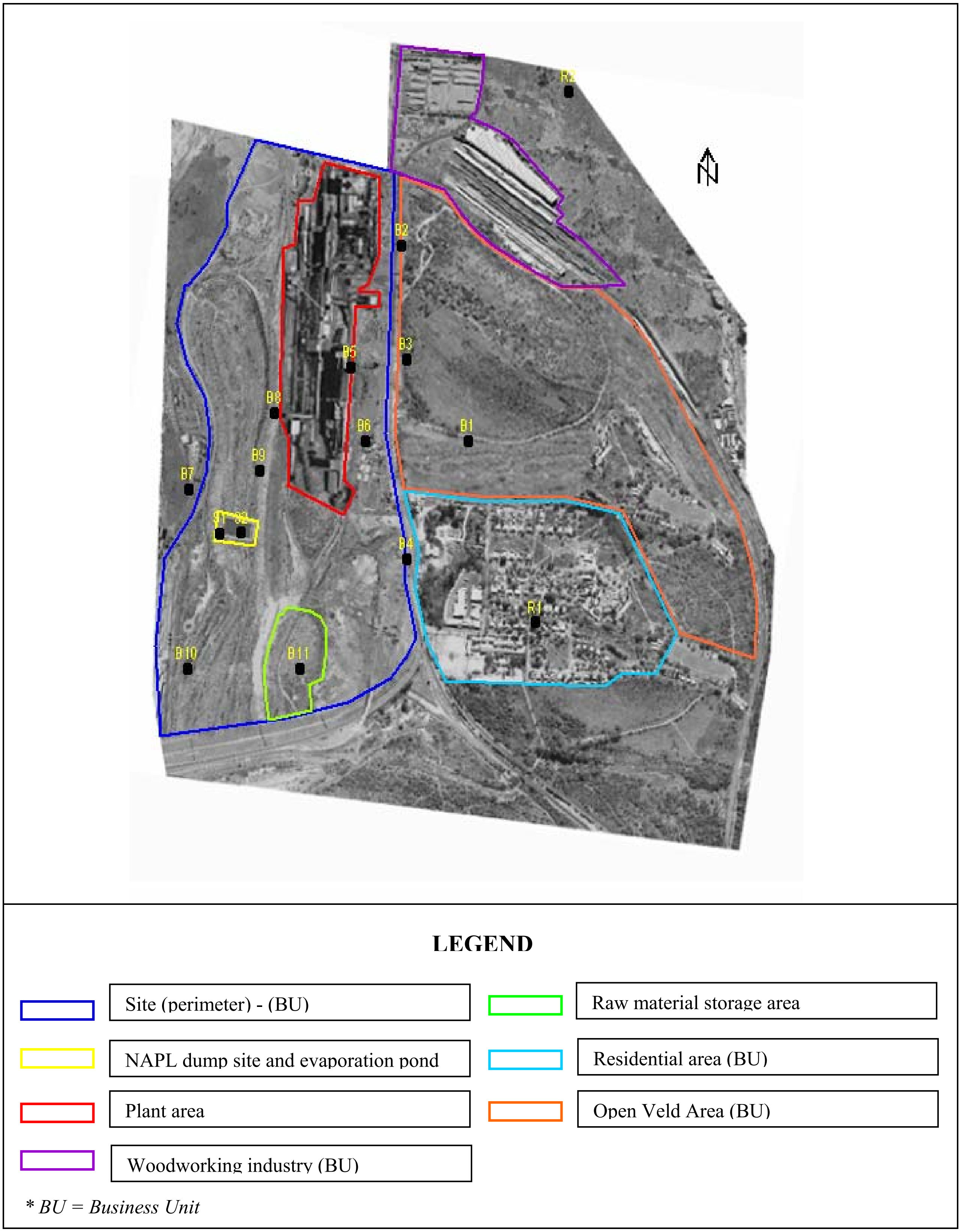


Figure 7-30 (Aspect map)

The aspect and impact register is described in **TABLE 7-10,** for each of the business units. Aspects that might have an impact in a particular business unit are highlighted and the type of impact described under "Impact type". The business units and aspects have been divided into sources and receptors.

TABLE 7-10

Business Unit	Aspect	Source / Receptor	Impact type	Impact chemicals
Site	Plant	Source	Coke-, blast-, and steel furnaces - Oily runoff, coke dust, slag	Phenols, BTEX, creosote
	Raw product storage area	Source	Rainfall infiltration, dissolution metals into groundwater	Fe, Mg, SO4
	NAPL Dump site and evaporation pond	Source	NAPL stored in drums underground – leaks. Evaporation pond leachate. Slag	Phenols, BTEX, creosote
Woodworking industry	Unkown	Source - other	Possibly runoff from plant, sawmill dust	Phenols
Residential area	None	Receptor	Impact on receptor from the site.	Fe, Mg, SO4, phenols
Open veld area	None	Receptor	Impact on receptor from site	Fe, Mg, SO4, phenols

DEAT (2002) has described an impact assessment protocol, which will be applied in the impact assessment.

7.3.3 Impact assessment

The following generic criteria have been drawn from the published literature and South African practice as prescribed by DEAT (2002). Some of the criteria, as applicable to groundwater and this site, will be used to describe the magnitude and significance of the impacts. Criteria highlighted in red are active components used for this impact assessment, and criteria in green are inactive components (i.e. not used for this impact assessment). The criteria are:

- Extent or spatial scale of the impact (In this case study adjusted to reflect the 'local scale of impact', see section 3.1 – **TABLE 7-9**).
- Intensity or severity of the impact (which will be adjusted for the groundwater case study)
- Duration of the impact
- Mitigatory potential
- Acceptability
- Degree of certainty
- Status of the impact
- Legal requirements (not applied in this case study)

Impact ratings will be assigned for each criterion, which are listed below:

Extent or spatial scale of the impact (Local scale of the impact)

Rating	**Comment**
Low:	Impact located around the source(s)
Medium:	Impact covering part of the investigated site but does not extend beyond the site boundaries
High:	Impact extends beyond the site boundary

Intensity or severity of the impact

Rating	**Comment**
High:	More than 50% of a specific constituent's values for site boreholes above the non-compliant MSWQS standard
Medium:	20 to 50% of the constituent values show marginal / non-compliance in terms of the MSWQS standard.
Low:	Less than 20% of the constituent values show marginal / non-compliance in terms of the MSWQS standard.

Duration of the impact

Rating	**Comment**
High (Long term):	Permanent. Beyond decommissioning. Long term (more than 15 years).
Medium (Medium term):	Reversible over time.

	Lifespan of the project. Medium term (5 – 15 years).
Low (Short term):	Quickly reversible. Less than the project lifespan. Short term (0 – 5 years).

<u>Mitigatory potential</u>

Rating	**Comment**
High:	High potential to mitigate negative impacts to the level of insignificant effects.
Medium:	Potential to mitigate negative impacts. However, the implementation of mitigation measures may still not prevent some negative effects.
Low:	Little or no mechanism to mitigate negative impacts.

<u>Acceptability</u>

Rating	**Comment**
High (Unacceptable):	Abandon project in part or in its entirety. Redesign project to remove impact or avoid impact.
Medium (Manageable):	With regulatory controls. With project proponent’s commitments.
Low (Acceptable):	No risk to public health.

<u>Degree of certainty</u>

Rating	**Comment**
Definite:	More than 90% sure of a particular fact. Substantial supportive data exist to verify the assessment.
Probable:	Over 70% sure of a particular fact or of the likelihood of that impact occurring.
Possible:	Only over 40% sure of a particular fact or of the likelihood of an impact occurring.
Unsure:	Less than 40% sure of a particular fact or the likelihood of an impact occurring.

Additional categories

The following additional categories can also be used:

Status of the impact
Specialists should describe whether the impact is positive (a benefit), negative (a cost) or neutral. (This category has been applied in the impact assessment of this case study)

Legal requirements
Specialists should identify and list the specific legal and permit requirements that could be relevant to the proposed project. (Not applied in this case study).

The above criterions have been applied to set up a contaminant impact matrix, as shown in **TABLE 7-11**. These impact ratings describe only the impact and should not be confused with the definition for risk as described in Chapter 2. Risk assessment of these values will follow in Chapter 8.

TABLE 7-11

	Extent or spatial scale (Local scale of the impact)	Intensity or severity of the impact	Duration of the impact	Mitigatory potential	Acceptability	Degree of certainty	Status of the impact
Naphthalene	High	High	High	Low	Medium	Probable	Negative
Benzene	Medium	High	High	Low	Medium	Probable	Negative
m-Xylene	High	Medium	High	Low	Medium	Probable	Negative
Ethylbenzene	Medium	Medium	High	Low	Medium	Probable	Negative
Tetrachloroethene	Medium	Medium	High	Low	Medium	Probable	Negative
Chloroform	High	Medium	High	Low	Medium	Probable	Negative
Phenol	Low	Medium	High	Low	Medium	Probable	Negative
Acenaphthene	High	High	High	Low	Medium	Probable	Negative
Phenanthrene	Medium	High	High	Low	Medium	Probable	Negative
Anthracene	Low	Medium	High	Low	Medium	Probable	Negative
Fluoranthene	Low	Medium	High	Low	Medium	Probable	Negative

Values have been assigned to the impact ratings above, in order to determine the total combined impact. The values have been assigned in such a manner that high values will reflect negative scenarios and low values positive scenarios. The values assigned, can be seen on the next page.

For *Local scale of the impact (Extent or spatial scale of the impact*), *Intensity or severity of the impact, Duration of the impact* and *Acceptability* the following values:

Low = 1
Medium = 2
High = 3

For *Mitigatory potential* the following values:

Low = 3
Medium = 2
High = 1

For *Status of the impact* the following values:

Neutral = 0
Negative = 3

For *Degree of certainty* the following values:

Definite = 3
Probable = 2
Possible = 1
Unsure = 0

These values have are shown in **TABLE 7-12**, and the median was calculated for all the categories shown in **TABLE 7-12**. This mode represents the final rating.

TABLE 7-12								
	Extent or spatial scale (Local scale of the impact)	Intensity or severity of the impact	Duration of the impact	Mitigatory potential	Acceptability	Status of the impact	Degree of certainty	Mode / Final Rating
Naphthalene	3	3	3	3	2	3	2	3
Benzene	2	3	3	3	2	3	2	3
m,p-Xylene	3	2	3	3	2	3	2	3
Ethylbenzene	2	2	3	3	2	3	2	2
Tetrachloroethene	2	2	3	3	2	3	2	2
Chloroform	3	2	3	3	2	3	2	3
Phenol	1	2	3	3	2	3	2	2
Acenaphthene	3	3	3	3	2	3	2	3
Phenanthrene	2	3	3	3	2	3	2	3
Anthracene	1	2	3	3	2	3	2	2
Fluoranthene	1	2	3	3	2	3	2	2
							Mode	3

Derivation of the final rating:

The final rating has been derived by calculating the mode of each chemical variable, and then calculating a single final mode from the mode values which were calculated for each variable. In a set of values, the mode is the most frequently occurring value (Steyn *et al*, 2000).

The Final rating value weights listed in TABLE 7-21 were each given Final Impact Status descriptions, which can be seen below:

Final Rating value	*Final Impact Status*
1	Low
2	Medium
3	High

The final mode value returned was a 3. It can thus be concluded from the above data that the final impact status reflects a large impact. Risk assessment will be performed in Chapter 8 to determine the associated risk and from that the desired action to be taken regarding this contaminated site.

7.4. CONCLUSIONS

In performing site assessment and characterization, the following problems were encountered and need to be addressed by groundwater practitioners, the industry and regulators:

- The industry needs to keep good record of their actions on site, any building up or breaking down of works on site, where contaminant materials are moved and stored. All the process wastes must be identified and a final acceptable destination should be determined for each process waste.

- Following from the above conclusion, regulators should put regulations in place for manners in which to handle different industries and the wastes associated with each industry. The industries should be ranked in terms of their contribution towards organic pollution and the industries should be addressed accordingly.

- Groundwater practitioners should address problems such as determining apertures accurately in fractured rock environments since aperture sizes will govern the flow dynamics of NAPL and is one of the determining factors in fractured rock flow. The accurate determination of saturation should also be addressed. Much work still needs to be done in site characterization, in determining what the most cost effective ways are to perform site characterization, but that still answers the questions that need to be answered for risk assessment and site remediation.

Chapter 8

Risk Assessment

8.1 INTRODUCTION

Soil and groundwater contamination and remediation problems exist worldwide. An estimate made in 2001 lists the following statistics of contaminated sites: 50 000 sites in Germany, 110 000 sites in The Netherlands, 9 000 sites in Denmark and 200 000 (+) ha in the United Kingdom. The cost of remediation could easily exceed 10 000 million pounds. (Khan and Husain, 2001)

Quantifying real risk would enable a more cost-effective and targeted response to contaminated site problems. This chapter will discuss tools for risk assessment and continue the impact assessment with the fictitious site.

8.2 WHAT IS RISK ASSESSMENT?

Risk assessment is a method of organizing information to support risk-based decisions for managing risks to human health and the environment. Risk assessment uses the best available scientific evidence (and data gap filling default assumptions) to estimate risks of an undesirable impact in a given situation. These results are used to manage risks in ways that meet social goals. Several risk assessment guidelines exist, of which the RBCA (EPA) and the R&D (Environment Agency, UK) will be discussed in section 8-3. While most formal quantitative risk assessment procedures organize information into four steps, two are of primary importance (Khan and Husain, 2001), which are 1) *Assessment of exposures* and 2) Understanding how undesirable impacts (diseases) are related to various exposure levels (*Dose response / toxicity assessment*).

Exposure Assessment consists either of direct measurement of exposure levels at receptors (e.g. concentrations of contaminants in water ingested) or model result predicting the exposure levels currently occurring or likely to occur in future. Typically the exposure assessment includes the measurement of current exposure levels as well as the estimate of future exposure levels and durations. *Dose-Response (Toxicity) Assessment* uses the best available evidence from human and animal studies to estimate the likelihood and severity of impacts that can be expected from the exposure levels (and durations) expected to be present in a given situation.

In summary, risk assessment includes both estimates of the exposure levels and the outcomes that could be expected at those exposure levels. Quantitative risk assessment can be a simple observation or estimate of contaminant concentrations at a receptor and the comparison of that exposure value to reference levels deemed to be acceptable for lifetime exposures (Khan and Husain, 2001).

8.3 DESCRIPTION OF THE DIFFERENT RISK ASSESSMENT PROCEDURES EXISTING WORLDWIDE

RBCA (EPA):

The Comprehensive Environmental Response, Compensation and Liability Act (CERCLA) and the Resource Conservation Act (RCRA) in the United States of America require the remediation of hazardous waste sites. In response the Risk Based Corrective Action (RBCA) is a concept that was developed by the American Society for Testing Materials (ASTM) to determine effective remediation targets. The development of the RBCA was the first formalization of the use of the risk based remediation strategy.

The formal EPA definition of RBCA is - *A streamlined approach in which exposure and risk assessment practices are integrated with traditional components of the corrective action process to ensure that appropriate and cost-effective remedies are selected, and that limited resources are properly allocated.* RBCA is a tiered approach to the assessment of cleanup, as is represented by the flow chart below, depicting the overall process:

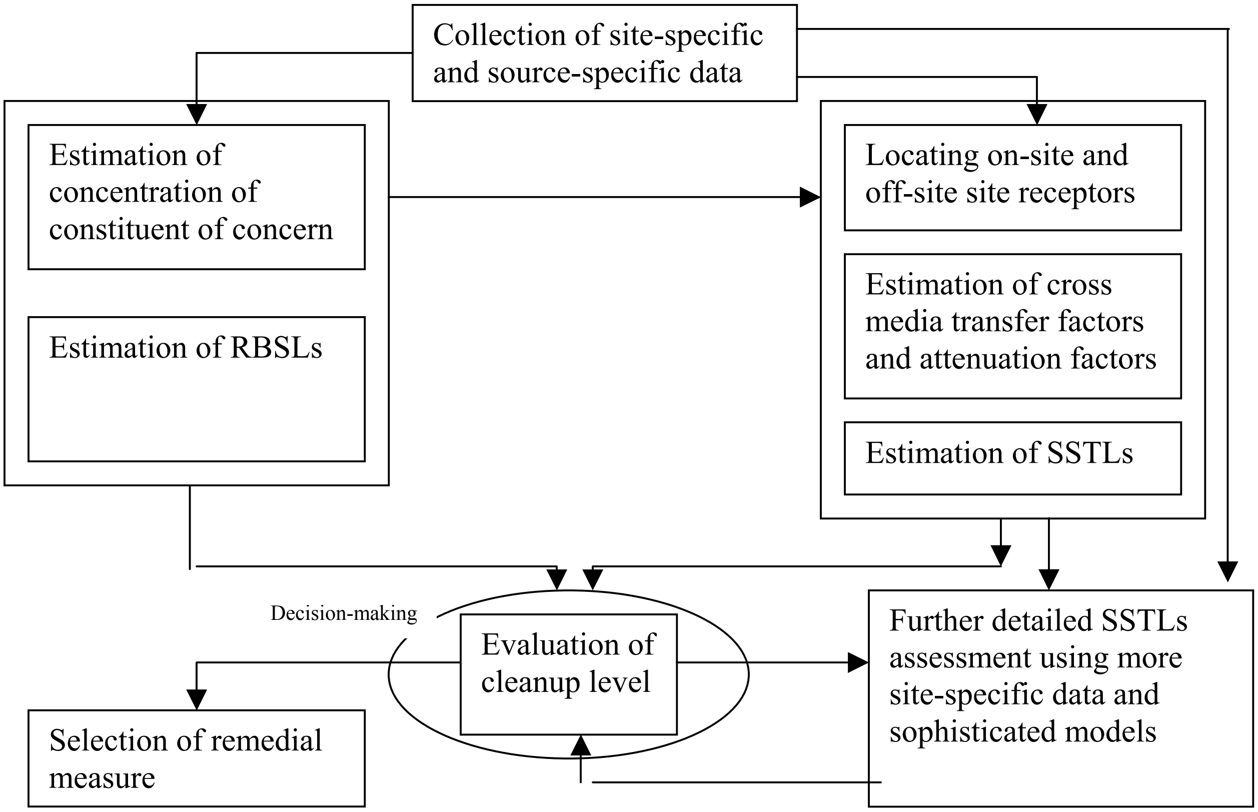


Figure 8-1: (RBCA flow chart (Khan and Husain, 2001))

The different Tiers will be described below (information obtained from Khan and Husain, 2001)

Tier 1:

This involves a traditional site assessment based on source characterization, the potential for exposure, the extent of contaminant migration and a summary of the site characterization results. Contaminant concentration levels are compared with risk based screening levels (RBSLs) derived from conservative default fate and transport and risk assessment parameters. If the results of a Tier 1 (based on conservative parameters) assessment are unacceptable due to cost or feasibility considerations, additional site information can be obtained according to Tier 2 criteria.

Steps:

1. Preliminary site assessment
2. Compare site to conservative Risk-Based Screening Levels (RBSL's)
3. Classification of urgency of initial response. If RBSL's are exceeded (in California maximum contaminant levels ((MCL's) for groundwater) go to Tier 2

Tier 2:

This involves the use of site-specific data (instead of Tier 1 default levels) to develop site-specific target levels (SSTLs), based on the site's relevant physical and chemical characteristics, augmented by the analytical fate-and –transport and risk assessment modeling. This measures migration and attenuation of contaminant from the source areas. Tier 1 RBSLs and Tier 2 SSTLs represent concentration limits within the source zone. SSTLs differ from RBSLs in three significant ways, however:

- Site-specific data is used to calculate risk based cleanup goals
- Human exposure to affected media may occur not only at the source zone, but as a separate point of exposure; and
- The effects of natural attenuation on constituent concentrations during lateral transport from the source to an off-site point of exposure are considered in the SSTL calculation.

Steps:

1. Develop risk-based Site-Specific Target Levels (SST's)
2. Select remedy to obtain SSTL's
3. Or perform more detailed Tier 3 evaluation

Tier 3:

If Tier 2 remedial measures are unacceptable, assessment can be done according to Tier 3 assessment criteria. Tier 3 involves a further expanded site assessment with SSTLs based on sophisticated statistical, fate-and-transport and risk assessment models. Models for Tier 3 is highly complex and the data requirement highly specific, without a significant improvement in the predictions.

Steps:
1. More site data, more evaluation.

Moving from Tier 1 to Tier 3:

- Each level becomes less generic
- Each level becomes less conservative
- Each tier has the same objective – compliance with a level of acceptable risk
- Each tier offers the same level of health protection.

R&D (Environment Agency, 1999):

This approach provides a methodology for the derivation of the level of remediation required to protect groundwater and calculate the risk represented by the contaminant source. The methodology is based on a risk assessment approach and incorporates a source-pathway-receptor analysis that leads to the derivation of remediation criteria based on an assessment of the potential impact at the identified receptor.

The procedure for determining site-specific remedial targets is summarized as follows:

- Determine a target concentration at the receptor or compliance point in relation to its use.
- Undertake the tier assessment (soils) to determine whether the contaminant source would result in the target concentration being exceeded at the receptor or compliance point. A remedial target is determined at each tier.
- The assessment in relation to contaminated groundwater commences at **Tier 3** and the only significant processes are attenuation, dispersion and further dilution as the groundwater moves from the source to the receptor.

8.4 RISK ASSESSMENT IN SOUTH AFRICA

Currently no guideline exists *per se* in the South African enviro-legal context, by which risk assessment is to be performed. This implies that risk assessment guidelines from other countries have to be adapted if needed, and used for risk assessment in South Africa. The DWAF is in the process of developing a risk assessment protocol (Bredenhann, 2004)

Seeing as the DWAF puts specific emphasis on the source-pathway-receptor principle, the Environmental Agency gives the best guidance on how to perform a risk assessment in the South African context. The Environment Agency also takes cost implications into account. The interaction of these three aspects is especially important when assessing risk of pollution, since different sources of pollution will have different impacts on different environments. Risk is only implied where there is a link between the source, pathway and receptor. If the link is broken, no risk is posed. Any artificial introduction of substances to the environment could be considered as a sustainable use (after risk analysis has been performed on it) and then only when the level of exposure reaches a certain determined limit, this contamination will be considered as pollution.

To follow an example of risk assessment and the derivation of remedial targets will be given, by following the R&D approach and data from the hypothetical site described in Chapter 7. An *Exposure Assessment* (see section 8-5) will be performed, using the R&D approach from the Environment Agency (1999), and a *Dose-Response (Toxicity) Assessment* (see section 8-6) will be performed, using risk to the environment and human health maximum contaminant levels, as obtained from South African toxicologists.

8.5 CASE STUDY - EXPOSURE ASSESSMENT (ENVIRONMENT AGENCY'S R&D APPROACH)

Specific equations related to the approach: Groundwater remedial targets derivation approach:

Tier 3 considers whether natural attenuation of the contaminant takes place and if it is sufficient to reduce contaminant concentrations at the receptor to acceptable levels. Tier 3 uses simple analytical models to calculate the significance of natural attenuation.

$$AF \text{ (Attenuation Factor)} = C0 / CT \qquad \textit{Equation 8-1}$$

C0 = Contaminant concentration in groundwater below source (mg/l)
CT = Contaminant concentration at target (mg/l)

And the remedial target (LTC_2) is determined as follows:

$$LTC_2 = C_T \times AF \qquad \textit{Equation 8-2}$$

The simulated compliance point concentration is determined by the either the Domenico equation (**Equation 8-3**) or the Ogata-Banks equation (**Equation 8-4**):

$$C_{ED} = C_0 \exp\left\{\frac{x}{2a_x}\left(1-\sqrt{\left[1+\frac{4\lambda a_x}{u}\right]}\right)\right\}.erf\left\{\frac{S_y}{2\sqrt{a_y x}}\right\}.erf\left\{\frac{S_z}{4\sqrt{a_z x}}\right\} \qquad \textit{Equation 8-3}$$

$$
\begin{aligned}
C_{ED} = \frac{C_0}{8} & \exp\left\{\frac{x}{2a_x}\left(1-\sqrt{\left[1+\frac{4\lambda a_x}{u}\right]}\right)\right\}.erfc\left\{\frac{1}{2\sqrt{a_x ut}}.\left(x-ut\sqrt{\left[1+\frac{4\lambda a_x}{u}\right]}\right)\right\} \\
& + \exp\left\{\frac{x}{2a_x}\left(1+\sqrt{\left[1+\frac{4\lambda a_x}{u}\right]}\right)\right\}.erfc\left\{\frac{1}{2\sqrt{a_x ut}}.\left(x+ut\sqrt{\left[1+\frac{4\lambda a_x}{u}\right]}\right)\right\} \\
& .\left[erf\left\{\frac{z+\frac{S_z}{2}}{2\sqrt{a_z x}}\right\}-erf\left\{\frac{z-\frac{S_z}{2}}{2\sqrt{a_z x}}\right\}\right].\left[erf\left\{\frac{y+S_y}{2\sqrt{a_y x}}\right\}-erf\left\{\frac{y-S_y}{2\sqrt{a_y x}}\right\}\right]
\end{aligned}
\qquad \textit{Equation 8-4}
$$

Equation 8-3 reflects the Domenico equation for steady state and vertical dispersion and advection in one direction. **Equation 8-4** reflects the Ogata-Banks equation for vertical dispersion and advection in one direction. Other variations are the Domenico steady state for vertical dispersion in two directions, and the Domenico time variant for vertical dispersion and advection in one and in two directions. These can be seen in the Remedial Targets Worksheet v2.2a: User Manual, 2001.

Other relevant equations that are used in the determination of the concentration of the contaminant at distance (CED), are:

Retardation factor:

$$Rc = (1 + \frac{K_d \rho}{n}) \qquad \textit{Equation 8-5}$$

Rate of contaminant movement due to retardation:

$$U = \frac{Ki}{nR_c} = \frac{Ki}{n + K_d \rho} \qquad \textit{Equation 8-6}$$

Where

CED = concentration of contaminant at distance

C0 = initial contaminant concentration in groundwater (mg/l)

λ = decay constant = 0.639 / half life for degradation of contaminant in days

ax, ay, az = dispersion coefficient in three dimensions (m)

Sz, Sy = width and thickness of plume at source

Rc = retardation factor

Kd= partition coefficient (l/kg)

ρ = bulk density (g/cm3)

n = effective porosity

I = hydraulic gradient

K = hydraulic conductivity

x = distance to compliance point (m)

y = Distance (depth) to compliance point perpendicular to flow direction (m)
z = Distance (lateral) to compliance point perpendicular to flow direction (m)
t = time (in days) since contaminant entered groundwater
Erf = error function
Erfc = complementary error function
Exp = Exponential

Case study:

The case study presented in Chapter 7, on which an impact assessment was performed, will be used to perform a risk assessment on.

Site information:

During the site characterization phase, a hydro-census was performed in order to assess what downstream users exist on whom the contaminated groundwater could impact. These are the receptors. The groundwater flow direction, velocity and path were determined which represent the pathway. Lastly the source was characterized in order to represent the source. In order for a risk to exist, a link must exist between the source, pathway and receptor. No barrier exists between the source and the receptor, and the pathway is groundwater flow via the matrix and fractures.

The source:

Represented by the raw material storage area, NAPL dump site and the plant area. Constituents from the source causing pollution (occurring past the site boundary) and possibly posing an environmental and human risk, are acenapthene, chloroform, m-xylene and naphthalene. Dissolved phase NAPL values were used.

The pathway:

The pathway is the aquifer, and groundwater flows via the matrix and fracture networks towards the receptor. The flow direction is towards the northeast (along the topography) and towards the east (along the dyke representing a preferential pathway). The general flow velocity has been determined as follows (see next page):

$$v = \frac{K \times i}{n}$$

Equation 8-7

where:
v = groundwater velocity
K = hydraulic conductivity (m/day) = 0.03 *m/d*
i = hydraulic gradient = 0.04
n = effective porosity = 0.03 (3%)

Substituting the given values: $v = \dfrac{0.03 \times 0.04}{0.03} = 0.04$ *m/d* or 14.6 *m/a.*

** Given values form part of the hypothetical case study site characterization.*

The receptor:

The receptor has been identified as external user boreholes downstream from the source areas. Two boreholes have been identified:

100m

R1 A residential borehole in the employee residential area used for watering the garden (no domestic use was reported)
R2 A regulatory authority monitoring borehole downstream of the low-impact wood re-working industry. The industry obtains it wood from a nearby pine plantation.

The site has been described and can be seen in **FIGURE 7-29** in Chapter 7.

The following boreholes were drilled:
BH1 – BH11 (Site characterization boreholes, future monitoring boreholes)
S1 – S2 (Source boreholes)

The following boreholes were receptor boreholes:
R1 – R2 (Receptor boreholes)

Determining Tier 3 Groundwater remedial targets

The R&D publication 20 Remedial Targets Worksheet, release 2.2a (Environment Agency, 2002) has been used to determine the remedial targets and receptor well concentrations after 9.9E+99 days.

Input options chosen for the R&D worksheet (note that various other options exist in the worksheet but that these were chosen for this specific case study and cannot be reflected in tabular format):

Analytical solution: The Ogata Banks equation was used for determination of the receptor well concentration, and steady state conditions were applied since variable time could result in over-optimistic receptor well concentrations.
Vertical dispersion: This was determined in two directions (up and down), which is consistent with the conceptual model of a source situated in the middle of the aquifer. For this case study, the source is assumed to be situated at the middle of the aquifer since organic pollution has been observed to be influenced by the fractures associated with the diabase intrusion, which means that pollution is already past the soil barrier associated with the topsoil and weathered zones. Upward dispersion from the fracture zones will probably occur.
Biodegradation rate: The option chosen was for degradation of the organic substance in water, since degradation rates from field studies was not available. A first order degradation process is assumed and

only contaminants in the aqueous phase will degrade, not those sorbed onto particles. Values from literature were used for degradation rates, of which the references are all cited in **TABLE 8-3.**

Partition coefficient: The Kd value has been determined for *non-polar* organic chemicals by the equation Kd = koc × foc (Pankow and Cherry, 1996), which is option 2 on the worksheet pull-down menu. Site-specific partition coefficients were not determined in the field.

Dispersivity: Dispersivity was calculated using Xu and Eckstein's (1995) equations.

Lateral distance to compliance point: This was set as zero to simulate a point located along the center line of the plume.

Depth distance to compliance point: This was set as zero to simulate a point located along the center line of the plume.

Time since pollutant entered groundwater: This was set as 9.9E+99 days in order to simulate steady state conditions and to avoid calculating overly optimistic remedial targets.

Measured pollutant value: The measured pollutant value is the average of boreholes S1 and S2 borehole groundwater measurements (**TABLE 8-2**).

The Tier 3 Target concentrations for each of organic variables (**TABLE 8-3**) have been determined using the variables given in **TABLE 8-1** (constant input parameters) and **TABLE 8-2** (chemical specific variables).

TABLE 8-1

Variable	**Value**
Sz (width of plume in m)	100
Sy (thickness of plume in m)	10
ρ (bulk density in g/cm^3)	1.65
n (effective porosity)	0.03
i (Hydraulic gradient)	0.04
k (Hydraulic conductivity in m/d)	0.03
z (Distance (lateral) to compliance point perpendicular to flow direction)	0
y (Distance (depth) to compliance point perpendicular to low direction)	0
t (Time since pollutant entered groundwater (days))	9.9E+99
x (Distance to compliance point in m)	50

TABLE 8-2

Variable	**Benzene**	**M-xylene**	**Ethylbenzene**	**Tetrachlorethene**	**Chloroform**	**Phenol**	**Naphthalene**	**Acenapthene**	**Phenanthrene**	**Anthracene**	**Fluoranthene**
Measured pollutant value (mg/L)	0.16	0.85	0.238	0.0735	1.326	3.95	36	0.0312	0.0312	0.02	0.014
Target concentration in groundwater (mg/l)	0.003	0.07	0.015	0.005	0.08	2	0.070	0.005	0.005	0.005	0.001
Half life	370 [1]	187 [1]	173 [1,2]	593.3 [1,3,4]	928 [1]	3.75 [1]	130 [1]	114 [1]	216 [1]	510 [1]	580 [1]
λ = decay constant = 0.639 / half life for degradation of contaminant in days	0.001727	0.00341	0.00369	0.00107	0.000689	0.1704	0.004915	0.005605	0.002958	0.001253	0.001102
Kd= partition coefficient (l/kg)	0.08778	0.129	0.204	0.265	0.0525	0.0288	1.191	4.898	11.261	23.4	49.269
Koc	87.78 [5]	129 [6]	204 [6]	265 [6]	52.5 [6]	28.8[6]	1191 [6]	4898 [6]	11261 [6]	23400 [6]	49096 [6]

[1] Howard *et al*, 1991

[2] Thierrin *et al*, 1995

[3] Thornton *et al,* 2000

[4] Vogel *et al*, 1987

[5] Spitz and Moreno, 1996

[6] Ohio, 2003

The results are shown in **TABLE 8-3**. The worksheets for each chemical can be seen in **APPENDIX D**.

TABLE 8-3

Variable	Benzne	M-xylene	Ethylbenzene	Tetrachlorethene	Chloroform	Phenol	Napthalene	Acenapthene	Phenanthrene	Anthracene	Fluoranthene
Receptor concentration (mg/L)	0.0199	0.0194	0.0042	0.019	0.546	9.27E-24	0.218	0.000107	0.0011	0.00422	0.00352
Remedial target (mg/L)	0.0242	3.08	0.852	0.094	0.195	8.55E+23	11.6	1.47	0.142	0.0238	0.00399

Orange: Representative of receptor well concentration nearing the remedial target value

Red: Representative of receptor well concentration above the remedial target value

Results:

Chloroform is one variable that shows concern, since the concentration at the receptor well is above the remedial target value. Remedial action is needed for this constituent. Benzene and tetrachlorethene approaches the remedial target value but do not exceed it. For all the other values the receptor concentrations are well below the remedial target values.

A note of caution should be made in terms of the Kd values determined for each of the constituents. In determining the Kd values, you use laboratory derived koc values – these parameters must be used with caution. The Ogata-Banks and Domenico equations used for the R&D worksheet, is also very sensitive to the half-lives used, and it is advised that the most accurate and conservative half-lives be used.

A shortcoming of this approach is that it does not determine the associated toxicity to human health and the environment. In order to address this problem, you can perform a dose response (toxicity) assessment (Section 8.6).

8.6 DOSE RESPONSE (TOXICITY) ASSESSMENT

The definition of dose response (toxicity) assessment is as follows: It uses the best available evidence from human and animal studies to estimate the likelihood and severity of impacts that can be expected from the exposure levels (and durations) expected to be present in a given situation (Khan and Husain, 2001). Measurements are made in terms of acute and chronic effects. Acute effects are easier to measure in the laboratory than chronic effects. The acute effects observed at certain doses of toxic substances, are used to create regulations regarding toxins (IET, 2004). Values used to determine the toxicity of samples analyzed for, has been obtained from the EPA (from various sites since one site usually does not have values for all the variables). Where toxicity values have not been found, maximum contaminant level (MCL) values were used. Currently no toxicity values exist in South Africa for human health, and although environmental values has been described and listed in the Waste Management Series (DWAF, 1998), these values were not used since it is currently under review. The new Minimum Requirements should be published early in 2005 and should have toxicity values for the environment as well as for human health. **TABLE 8-4** compares the groundwater analyses values with the toxicity values.

TABLE 8-4

Contaminant Grouping		VOC Top					SVOC Middle					
Variable (mg/l)		Benzene	m-xylene	Ethylbenzene	Tetrachlorethene	Chloroform	Phenol	Napthalene	Acenapthene	Phenanthrene	Anthracene	Fluoranthene
Boreholes	B1	DL	DL	DL	DL	DL	0.008	0.05	DL	DL	DL	DL
	B2	DL	DL	DL	DL	DL	0.01	0.04	DL	DL	DL	DL
	B3	DL	DL	DL	DL	DL	0.011	0.05	DL	DL	DL	DL
	B4	DL	DL	DL	DL	DL	0.01	0.04	DL	DL	DL	DL
	B5	0.009	0.076	0.015	0.001	0.029	0.129	13	0.015	0.013	DL	DL
	B6	0.017	0.088	0.015	0.003	0.031	0.19	10.2	0.015	0.017	DL	DL
	B7	DL	DL	DL	DL	DL	DL	0.175	DL	DL	DL	DL
	B8	DL	0.002	0.002	DL	DL	0.014	0.065	0.005	0.002	DL	DL
	B9	0.12	DL	DL	0.016	0.119	2.35	20.9	0.015	0.013	0.0115	0.003
	B10	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL
	B11	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL	DL
	R1	DL	0.041	0.007	DL	0.007	0.035	0.01	0.002	DL	DL	DL
	R2	DL	DL	DL	DL	DL	DL	0.008	DL	DL	DL	DL
	S1	0.2	1.13	0.234	0.082	1.163	4.2	47	0.0324	0.0324	0.022	0.01
	S2	0.116	0.57	0.242	0.059	1.489	3.7	25	0.03	0.03	0.018	0.008
Environmental Risk (mg/l) (a)		0.114	0.027	0.014	0.045	0.140	0.180	0.013	0.038	0.0036	0.000035	0.0019
Human Risk (mg/l)		0.005 (b)	10 (b)	0.7 (b)	0.005 (b)	0.343 (c)	22.289 (c)	0.323 (c)	1.435 (c)	0.005 (d)	5.333 (c)	0.75 (c)

Green: Representative Ecological Screening Level (ESL) values for the environment (chemical constituents in green is above this standard).

Red: Representative maximum contaminant level (MCL) values for human health (chemical constituents in red is above this standard).

Purple: Representative of chemical constituents above the ESL values for the environment and the MCL values for human health.

a – EPA (e), 2003; b – EPA, 2002; c – EPA, 2004; d – Wikipedia (Dutch Intervention values), 2004

The following conclusions can be made regarding the organic toxicity assessment:

- The following variables, in descending order of risk, were above the toxicity standards:
  Naphthalene (boreholes B5, B6 and B9, S1 and S2 in terms of both the human and ecological risk, B1-4, B7-8 in terms of ecological risk)
  Phenanthrene (boreholes B5, B6, B9, S1 and S2 in terms of ecological risk and human risk)
  Benzene (Borehole B9, S1 and S2 non-compliant in terms of human and ecological risk)
  Tetrachlorethene (borehole B9 – human risk, S1 and S2 both)
  Chloroform (boreholes S1 and S2 for both)
  Phenol (borehole B6, B9, S1and S2 in terms of environmental risk)
  Anthracene (borehole B9, S1and S2 in terms of environmental risk)
  Fluoranthene (borehole B9, S1and S2 in terms of environmental risk)
  M-xylene (borehole S1 and S2 in terms of environmental risk)

- The risk of naphthalene, phenanthrene, anthracene and fluoranthene are lowered due to the high sorption potential of these chemicals. This leaves benzene as one of the major chemicals of concern, followed by M-xylene, tetrachlorethene, chloroform and phenol.

- The toxicity assessment is not very accurate since toxicity values have not been determined yet for all values. In South Africa toxicity values have only been reported for the environment, as described in the Waste Management Series (DWAF, 1998). DWAF is currently, in association with South African toxicologists, busy updating the current toxicity values and will possibly add toxicity values for human health as well. As yet no permission for use or inclusion of these toxicology values in the thesis, have been obtained from the toxicologists approached.

In order to more clearly define the risk to human health, the RISC workbench model has been run on the same input parameters as the R&D method.

8.7 RISC WORKBENCH MODEL

The RISC Workbench model has been run on all the organic constituents in order to determine receptor concentrations.

The RISC model calculates what the concentration at the receptor will be, given a certain input concentration at the source. The same input parameters (see **TABLES 8-1** and **8-2**) were used in the RISC model and the output is given as change of receptor well contaminant concentration over time (**Figures 8-2** and **8-3**).

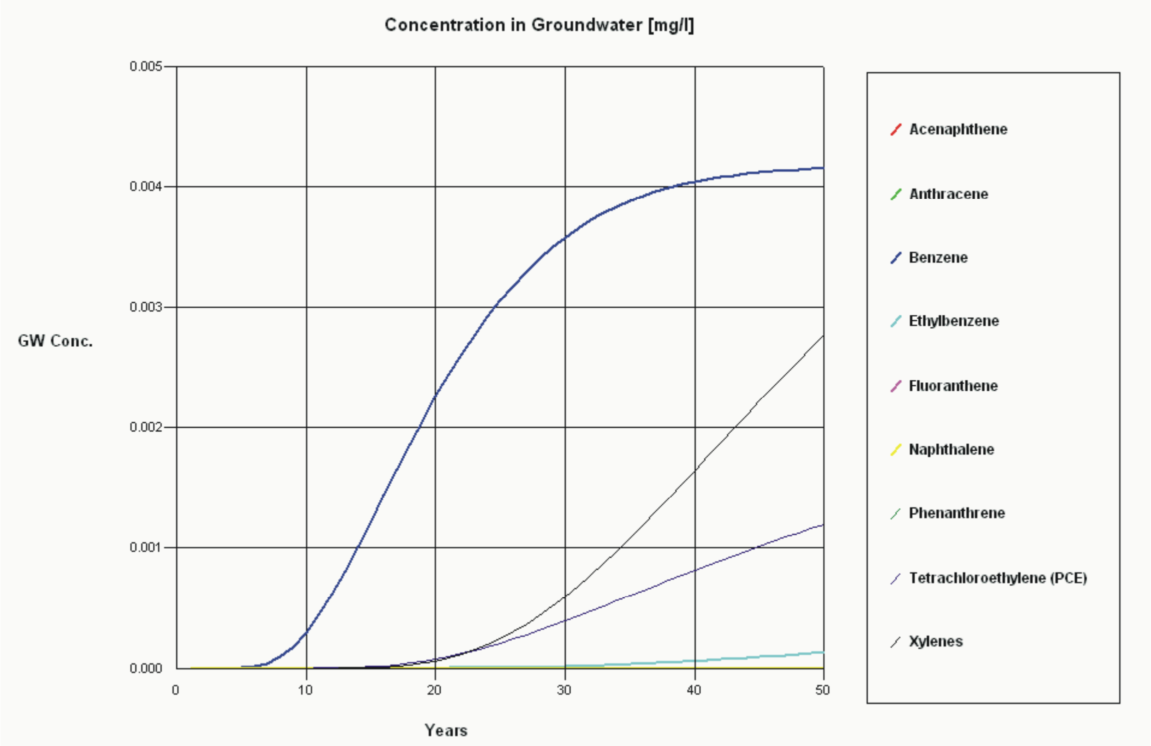


Figure 8-2 (Caption from RISC Workbench)

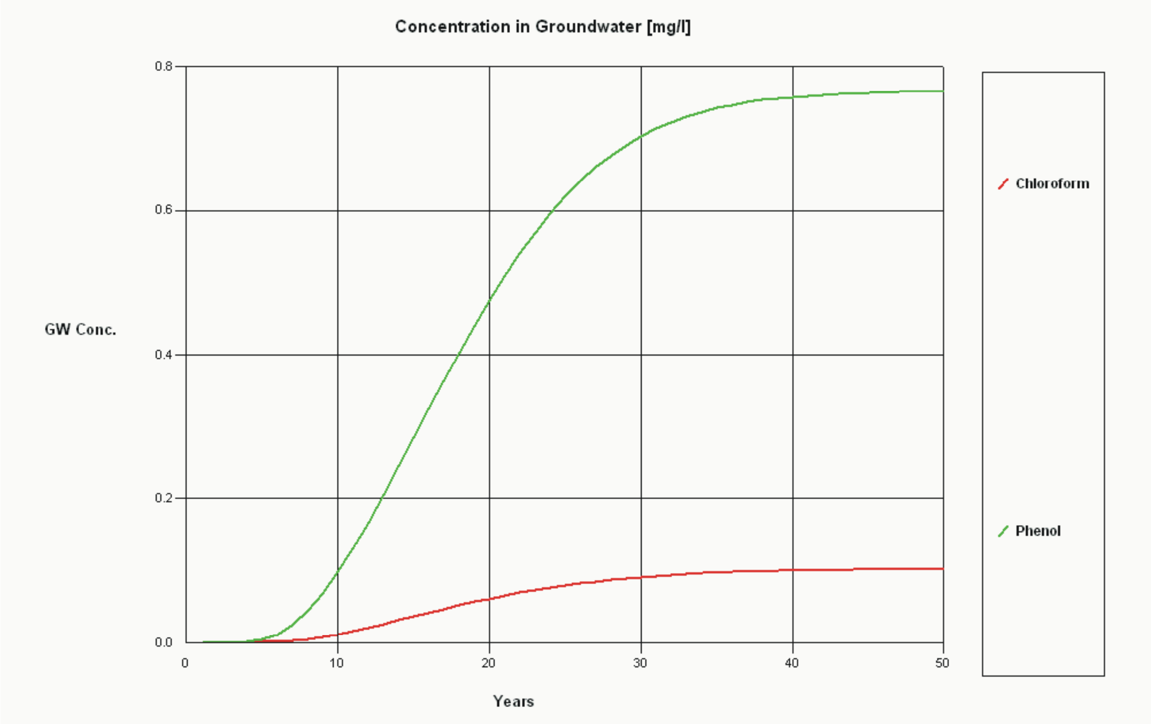


Figure 8-3 (Caption from RISC Workbench)

In **FIGURE 8-2** it can be seen that the receptor concentration for benzene will increase during a groundwater fate and transport model simulation time of 50 years to 0.00416 mg/L while naphthalene, acenapthene and anthracene's concentrations will not increase at the receptor at all. This is due to the fact that naphthalene is highly sorbed onto the soil and the retardation factor is thus very high. Chloroform and phenol have higher receptor well concentrations than the other chemicals have (**FIGURE 8-3**). The receptor well concentrations can be seen in the **TABLE 8-5**. Note: The exposure data for the two types of receptors simulated; was entered as receptor-specific data for the risk calculation of the receptors. These were as follows: Child resident: Bodyweight: 15 kg, lifetime: 70 years; and Adult resident: Bodyweight: 70 kg and lifetime: 70 years.

TABLE 8-5

Variable	Benzene	M-xylene	Ethylbenzne	Tetrachlorethene	Chloroform	Phenol	Naphthalene	Acenpathene	Phenanthrene	Anthracene	Fluoranthene
Receptor Well Concentration (mg/L)	4.16E-3	2.81E-3	1.34E-4	1.21E-3	1.01E-1	7.65E-1	1.49E-9	0	0	0	0

The only chemical that showed carcinogenic risk, is benzene, with a value of 3.3E-7 for a child, and 2.3E-7 for an adult. The total risk is 5.6E-7. This means that a risk exists that 5 persons in 10,000,000 may develop cancer, which is a low risk, and is generally accepted by experts worldwide.

The hazard index for each chemical has been determined and can be seen in **FIGURE 8-4** (next page). In the Risc Workbench program, the hazard index is defined as the sum of more than one hazard quotient for multiple chemicals and/or multiple exposure pathways, where the hazard quotient is the ratio of a single substance (chemical) exposure level over a specified time period to a reference dose for that substance. The hazard index values thus take into account multiple chemical effects.

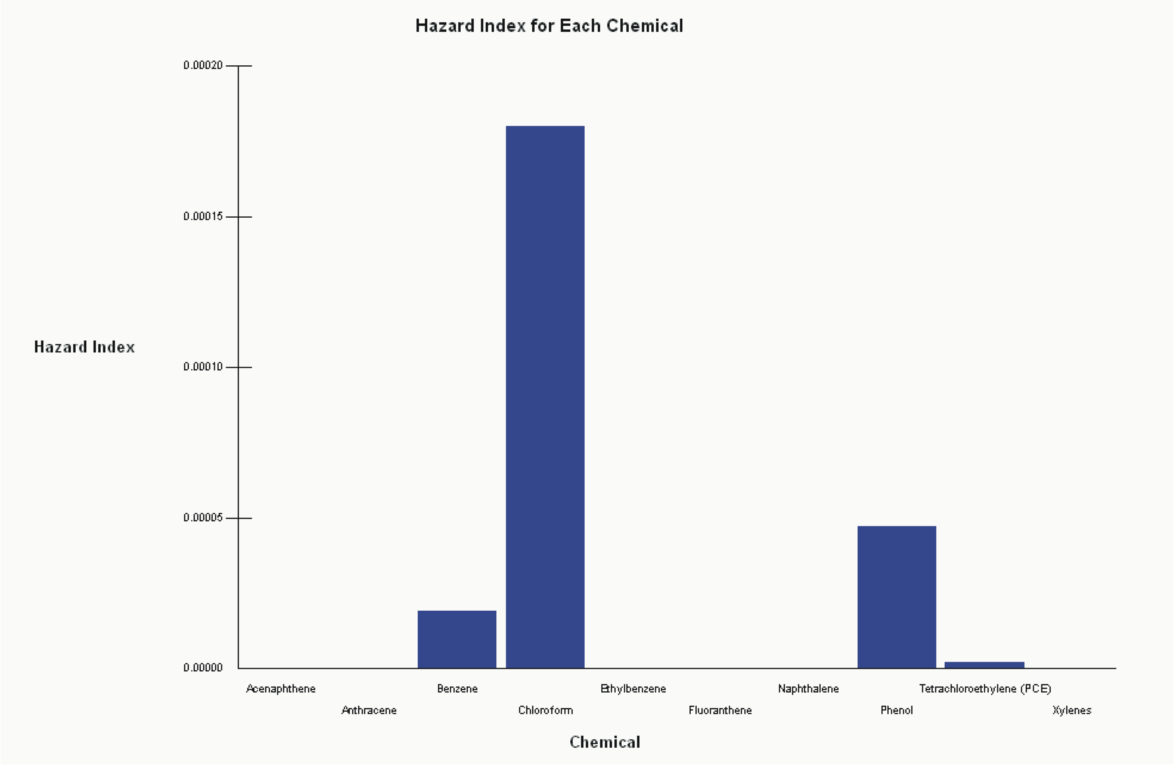
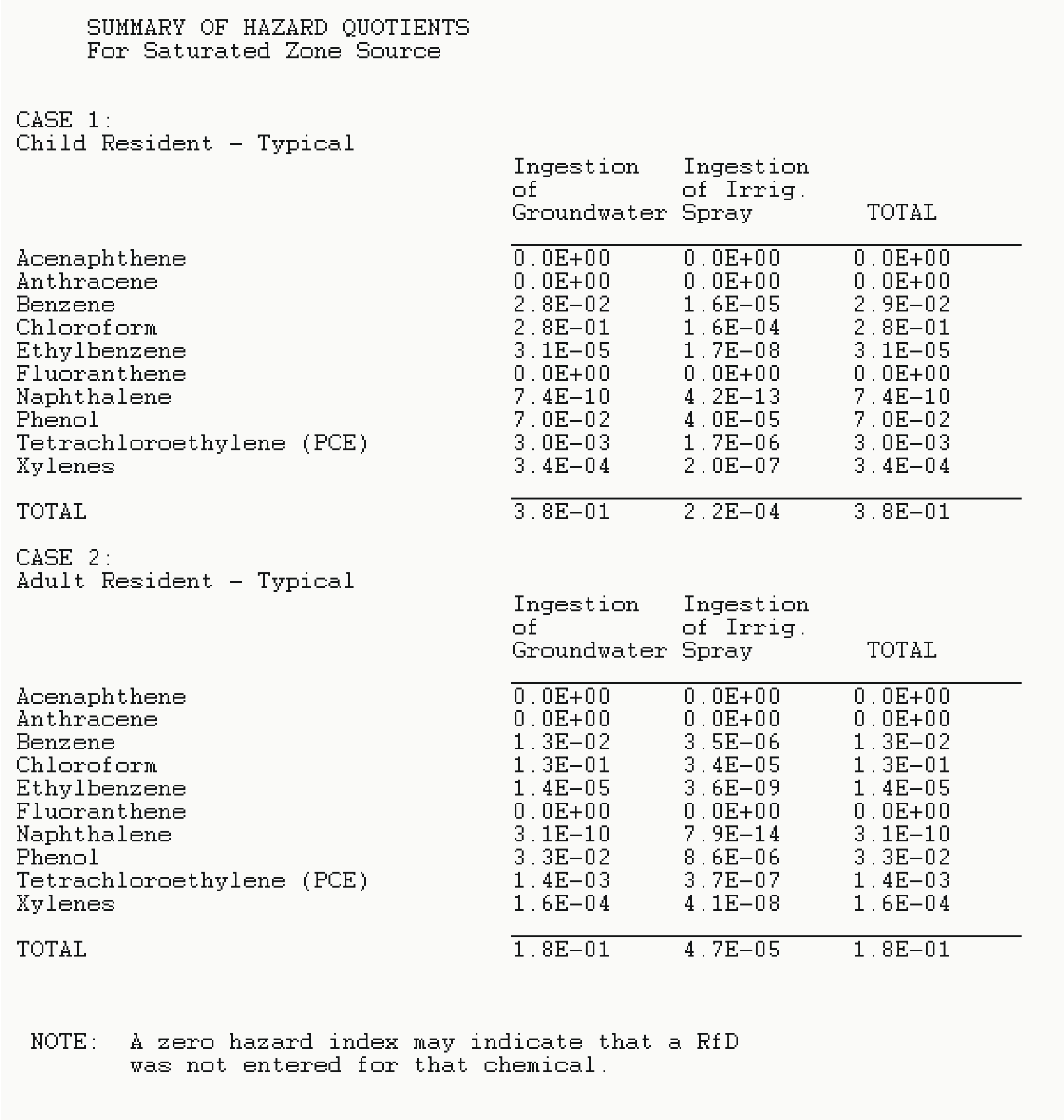


Figure 8-4 (Caption from RISC Workbench)

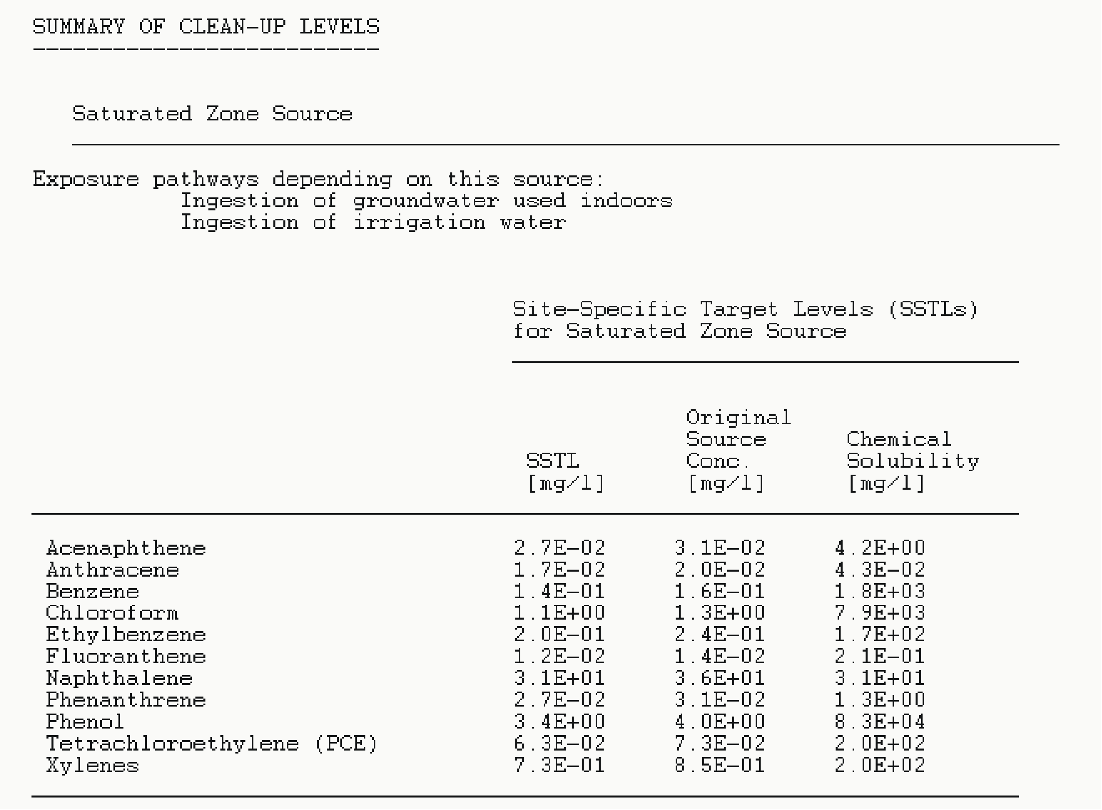
The hazard index values are as follows (captions from RISC Workbench):



```
     SUMMARY OF HAZARD QUOTIENTS
     For Saturated Zone Source


CASE 1:
Child Resident - Typical
                                   Ingestion   Ingestion
                                   of          of Irrig.
                                   Groundwater Spray        TOTAL
                                   ____________________________________
Acenaphthene                       0.0E+00     0.0E+00      0.0E+00
Anthracene                         0.0E+00     0.0E+00      0.0E+00
Benzene                            2.8E-02     1.6E-05      2.9E-02
Chloroform                         2.8E-01     1.6E-04      2.8E-01
Ethylbenzene                       3.1E-05     1.7E-08      3.1E-05
Fluoranthene                       0.0E+00     0.0E+00      0.0E+00
Naphthalene                        7.4E-10     4.2E-13      7.4E-10
Phenol                             7.0E-02     4.0E-05      7.0E-02
Tetrachloroethylene (PCE)          3.0E-03     1.7E-06      3.0E-03
Xylenes                            3.4E-04     2.0E-07      3.4E-04
                                   ____________________________________
TOTAL                              3.8E-01     2.2E-04      3.8E-01

CASE 2:
Adult Resident - Typical
                                   Ingestion   Ingestion
                                   of          of Irrig.
                                   Groundwater Spray        TOTAL
                                   ____________________________________
Acenaphthene                       0.0E+00     0.0E+00      0.0E+00
Anthracene                         0.0E+00     0.0E+00      0.0E+00
Benzene                            1.3E-02     3.5E-06      1.3E-02
Chloroform                         1.3E-01     3.4E-05      1.3E-01
Ethylbenzene                       1.4E-05     3.6E-09      1.4E-05
Fluoranthene                       0.0E+00     0.0E+00      0.0E+00
Naphthalene                        3.1E-10     7.9E-14      3.1E-10
Phenol                             3.3E-02     8.6E-06      3.3E-02
Tetrachloroethylene (PCE)          1.4E-03     3.7E-07      1.4E-03
Xylenes                            1.6E-04     4.1E-08      1.6E-04
                                   ____________________________________
TOTAL                              1.8E-01     4.7E-05      1.8E-01


 NOTE:  A zero hazard index may indicate that a RfD
        was not entered for that chemical.
```

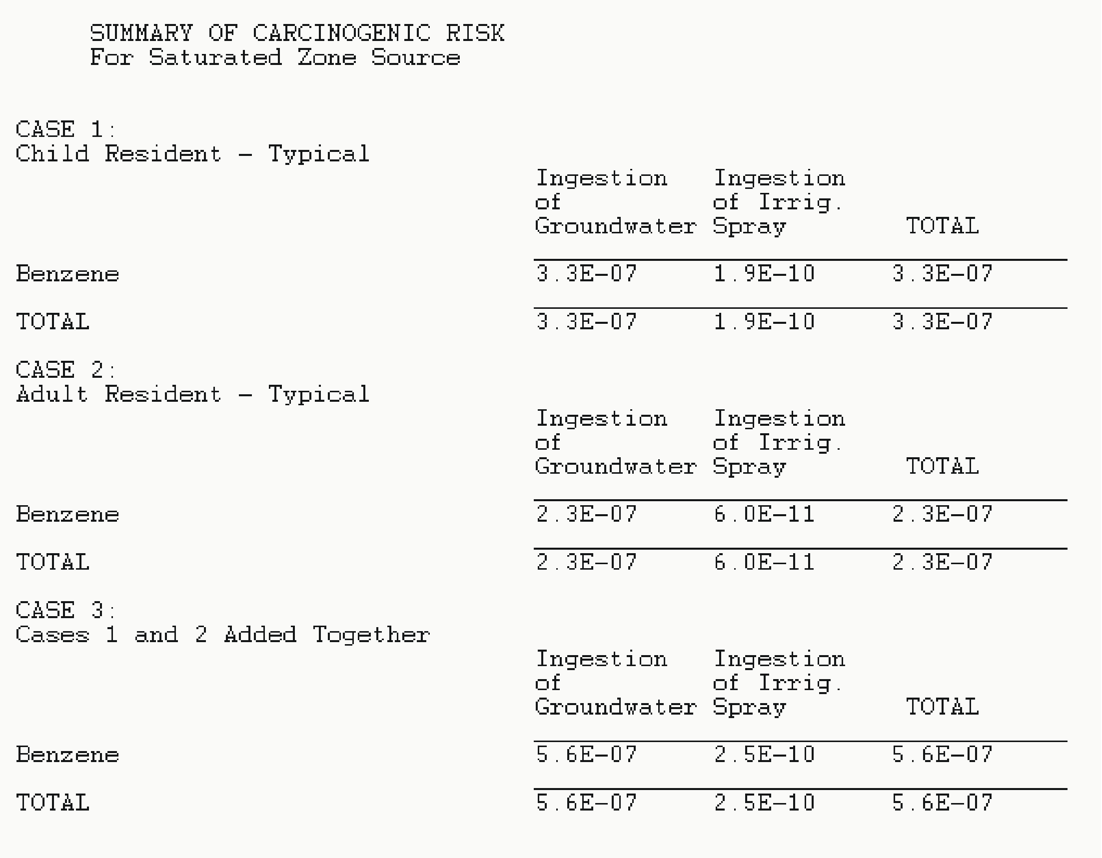
The cumulative risk for the child resident is 3.8E-1 and for the adult resident 1.8E-1. These are not above one and thus the values are within an acceptable range.

The clean-up levels (SSTL or Site-Specific Target Levels) have also been calculated for all the organic constituents:



```
SUMMARY OF CLEAN-UP LEVELS
--------------------------

   Saturated Zone Source
   ___________________________________________________________________________

Exposure pathways depending on this source:
           Ingestion of groundwater used indoors
           Ingestion of irrigation water


                                    Site-Specific Target Levels (SSTLs)
                                    for Saturated Zone Source
                                    ______________________________________

                                                Original
                                                Source      Chemical
                                     SSTL       Conc.       Solubility
                                     [mg/l]     [mg/l]      [mg/l]
___________________________________________________________________________

 Acenaphthene                       2.7E-02     3.1E-02     4.2E+00
 Anthracene                         1.7E-02     2.0E-02     4.3E-02
 Benzene                            1.4E-01     1.6E-01     1.8E+03
 Chloroform                         1.1E+00     1.3E+00     7.9E+03
 Ethylbenzene                       2.0E-01     2.4E-01     1.7E+02
 Fluoranthene                       1.2E-02     1.4E-02     2.1E-01
 Naphthalene                        3.1E+01     3.6E+01     3.1E+01
 Phenanthrene                       2.7E-02     3.1E-02     1.3E+00
 Phenol                             3.4E+00     4.0E+00     8.3E+04
 Tetrachloroethylene (PCE)          6.3E-02     7.3E-02     2.0E+02
 Xylenes                            7.3E-01     8.5E-01     2.0E+02
___________________________________________________________________________
```

Summary of carcinogenic risk:



```
     SUMMARY OF CARCINOGENIC RISK
     For Saturated Zone Source

CASE 1:
Child Resident - Typical
                                 Ingestion   Ingestion
                                 of          of Irrig.
                                 Groundwater Spray        TOTAL
                                 _________________________________
Benzene                          3.3E-07     1.9E-10     3.3E-07
                                 _________________________________
TOTAL                            3.3E-07     1.9E-10     3.3E-07

CASE 2:
Adult Resident - Typical
                                 Ingestion   Ingestion
                                 of          of Irrig.
                                 Groundwater Spray        TOTAL
                                 _________________________________
Benzene                          2.3E-07     6.0E-11     2.3E-07
                                 _________________________________
TOTAL                            2.3E-07     6.0E-11     2.3E-07

CASE 3:
Cases 1 and 2 Added Together
                                 Ingestion   Ingestion
                                 of          of Irrig.
                                 Groundwater Spray        TOTAL
                                 _________________________________
Benzene                          5.6E-07     2.5E-10     5.6E-07
                                 _________________________________
TOTAL                            5.6E-07     2.5E-10     5.6E-07
```

Conclusions regarding the RISC model:

The following conclusions can be made regarding the RISC model:

- The receptor well concentrations are the highest for phenol and chloroform, and the hazard index is the highest for chloroform, followed by phenol.
- Benzene was identified as the only chemical with carcinogenic risk (five in 10,000,000 persons run the risk of developing cancer).
- The cleanup level values of the RISC workbench and the R&D approach (remedial target values) as well as the receptor well concentrations calculated by each method, are compared in **TABLE 8-6.**

TABLE 8-6

Variable	**Remedial target (R&D)**	**Cleanup level (RISC Workbench)**	**Receptor well concentration R&D**	**Receptor well concentration RISC Workbench**
Benzene	0.0242	0.14	0.0199	0.00416
M-xylene	3.08	0.073	0.0194	0.00281
Ethylbenzene	0.852	0.2	0.0042	0.00013
Tetrachloethene	0.094	0.0063	0.019	0.00121
Chloroform	0.195	1.1	0.546	0.0101
Phenol	8.55E+23	3.4	9.27E-24	0.0765
Napthalene	11.6	31	0.218	1.49E-9
Acenapthene	1.47	0.027	0.000107	0
Phenanthrene	0.142	0.0027	0.0011	0
Anthracene	0.0283	0.017	0.00422	0
Fluoranthene	0.00399	0.0012	0.00352	0

The following conclusions can be drawn:

The correlation between the cleanup level values of the two methods is very small, with a correlation coefficient of 0.00466. A correlation coefficient of –0.04 is obtained if comparing the receptor well concentrations calculated with the two methods. A large contributing factor is the phenol calculation of the R&D method, of which the remedial target is notably larger than R&D and the receptor well concentration notably smaller. If phenol is removed from the correlation function, the correlation coefficient between the cleanup levels of the two methods is 0.96, while the correlation coefficient for the receptor well concentration calculations of the two methods is 0.804. Disregarding phenol, the correlation between the two methods is fairly high, when taking into account the variability of answers that the R&D method can produce since it is dependant on the input of values such as half-lives and koc values from the operator. Deciding on which values of the various values obtainable from literature, to use, is a daunting task. Koc values of laboratory studies have been reported to vary considerably (Spongberg and Gangliang, 2000), while half-lives also have various reported time spans, e.g. chloroform with a reported half-life of 928 days (Howard et al, 1991) versus 1760 years (Washington, 1995). A sensitivity analyses on the risk assessment parameters is recommended for future research, to determine where costs can be saved with cutting field experiments on relatively insensitive parameters.

8.8 URBAN RISK ASSESSMENT

The urban risk assessment model (IGS, 2004) as developed for the WRC, was also run, and as a representative for the case study, the other metal product manufacturing was selected as "source type".

At Tier 0, the total risk was calculated as 37%. The number of sources was low and the level of management also low (unsatisfactory)

At Tier 1, taking into account soil type, recharge etc, the following risks were calculated for benzene, ethylbenzene, chloroform and xylene. The other chemicals represented in the case study, were not listed under "other metal product manufacturing".

Tier 1 input parameters:
Recharge = 18 mm/a
Soil media = SaClLm-SaCl.
Aquifer media = fractured
Vadose zone = basalt
Groundwater depth = 5m
Topography slope = 3%

Tier 2 input parameters:
The chloride method was used to determine recharge and a recharge of 3% was determined.
The input for soil media, aquifer media, vadose zone, groundwater depth and topography slope is the same as in those for Tier 1.
Population size = range E (> 5000)
Exposure pathway = ingestion

The input parameters for each chemical's concentration is the same as given in **TABLE 8-3**. The results of Tier one and two can be seen in **TABLE 8-7**

TABLE 8-7				
	Benzene	**Ethylbenzene**	**Chloroform**	**Xylene**
Vulnerability	52	52	52	52
Health	99	25	75	25
Exposure duration	40	40	40	40
Source type	23	23	23	23
Physio-chemical	99	99	99	99
Total combined Risk Tier 1	62	47	57	47
Total combined Risk Tier 2	43	44	43	43

At a Tier 1 level, chloroform and benzene showed the highest risk, while at Tier 2 all of these contaminants showed relatively the same risk.

The health risk is the highest for benzene (a carcinogen), followed by chloroform. Ninety nine percent risk exists that people may become very ill from using the water with associated benzene levels while 75% risk exist that people may get very ill from using water contaminated with the levels of chloroform as entered into the URA program. The source type risk is relatively low for all contaminants, in that the contaminants have a 23% chance of reaching the groundwater resource.

According to the URA, the health risk is thus the highest for benzene and chloroform.

8.9 CONCLUSIONS

The following conclusions can be made regarding risk assessment in general:

Certain uncertainties exist regarding risk assessment, which is encountered during different stages of risk assessment, such as:

- deficiencies in toxicity and dose-response data (shown in Section 8.6 above);
- deficiencies in data for contaminant behavior in soils and groundwater (e.g. koc values, half-lives);
- unknown, but probable, interacting toxic effects resulting from exposure to multiple toxicants;
- validity of the exposure model and other assumptions made in extrapolating from test animals to humans and from high to low doses;

- variations in the magnitude of toxic effect(s) expressed among and within different age groups of a population from exposure to a given toxicant;
- difficulties in estimating the duration and intensities of life-time exposure(s) to various toxicants. (Rao *et al,* 2004)

Several generic datasets exist for values (i.e. foc values for certain types of soil, koc values for organic variables, retardation factors etc.), which could be used and referenced in risk assessments. Groundwater practitioners should, however, where possible, make measurements to obtain real data regarding a specific site in order to make the risk assessment conclusions as sound as possible. If data from literature is used, the various existing values should be compared in order to identify the most appropriate value, of which the repeatability of analysis has been established by published values that have a high correlation. A sensitivity analyses on the risk assessment parameters is recommended for future research, to determine where costs can be saved with cutting field experiments on relatively insensitive parameters.

South African toxicologists should make available toxicity standards for all missing / incomplete organic and inorganic constituents after taking into account all tests conducted up to date on animals and plants. At this stage a deficiency exists on human health toxicity data, as well as the interpretation and application of these values. Since these values are currently under review, permission was not granted to use these values in the thesis.

A comparison between the different risk assessment methods:

On a comparison between risk assessment using the R&D approach and RISC workbench, the following conclusions can be made:

- Chloroform was identified as the major chemical of concern with the R&D approach, with benzene and tetrachlorethene identified as chemicals of marginal concern. RISC workbench identified chloroform, phenol, benzene (a carcinogen) and tetrachlorethene as high hazard chemicals.
- During the R&D risk assessment and the toxicology comparisons, phenol did not present as a chemical of concern, which it did when the RISC model was applied.
- The two methods compare fairly well, except for the fact that phenol was not identified as a chemical of concern with the R&D method.
- The values for receptor well concentrations of the R&D and the RISC Workbench assessments differ, with the receptor well concentrations consistently lower for RISC Workbench than for R&D. It seems that the R&D assessment tool is more conservative than RISC Workbench.

To aid the R&D risk assessment, a dose response analyses was performed on the data, and chloroform, m-xylene, benzene, tetrachlorethene and phenol was identified as chemicals of concern. Napthalene, phenanthrene and anthracene was also highlighted, but these are rather immobile since they sorb strongly onto soil particles, and the associated risk was thus lowered. A good correlation exist between the *toxicity* *assessment* and the *exposure assessments* (R&D, RISC Workbench), but since these two approaches are entirely different tools, the toxicity assessment should not be used to replace an exposure assessment, but should be used in conjunction with exposure assessments, if the exposure assessment tool does not include a toxicity assessment.

Urban risk assessment was also performed and the following conclusions can be made:

At a Tier 2 level, chloroform and benzene showed the highest risk, while at Tier 3 all of these contaminants showed relatively the same risk. R&D and RISC Workbench also highlighted these two contaminants as contaminants of concern.

Not all variables that may be of concern associated with a certain source type are listed in the urban risk assessment program, but can be added. The program is a good first screening tool of the most highly expected contaminants. This program will therefore give a manager a good idea of what contaminants to expect in association with a certain industrial process. The program does not make use of the source-pathway-receptor principle when calculating risk, which the R&D method and the RISC workbench do take into account when calculating the risk of a certain chemical. In this respect, the urban risk assessment program may over-estimate risk and be too conservative in comparison with the R&D approach and the RISC Workbench program.

The Tier 2 risk percentages were constantly lower than the Tier 1 values. The screening level risk was lower than Tier 1 and 2, and may be due to the fact that site-specific values are not taken into account. The screening level risk (Tier 0) may thus be lower or higher than the site-specific tier 1 and 2 risk percentages.

What program is the best to use?

The answer to this question depends on the type of answer you want. If you want a screening level answer and are a typical manager that has to make a decision on a starting point for addressing a polluted site, the Urban Risk Assessment program would be the best answer. Typical questions that can be answered are: *What contaminants must be analyzed for associated with a certain industrial activity? What contaminants pose the highest health risk?* This program also specifically addresses risk in urban environments and have taken into account contaminants typically associated with certain sources in an urban environment. This is not an in-depth risk assessment tool and if the need is risk assessment on which decisions such as risk minimization measures and determination of the need of remediation or determination of remedial targets must be made, a program such as RISC Workbench must be used. This program takes into account the source, pathway and receptor (as does the R&D method), which is necessary when determining the real risk associated with a contamination source situated 100 m away from a receptor, as opposed to being 50 m away from a receptor. In this respect the URA may over-estimate the risk associated with certain chemicals.

The R&D approach is similar to RISC Workbench in that you can determine receptor well concentrations (given certain source concentrations) of a contaminant as well as the cleanup levels. The R&D approach has limitations in that the target concentrations and half-lives of the chemicals must be carefully chosen. The Kd values must be determined from measured *foc* values in order to calculate representative and accurate contaminant retardation factors. None of the solutions presented by the R&D methodology may be applicable to a highly heterogenous aquifer (a highly fractured aquifer for example). RISC Workbench also has built in hazard and toxicity assessments, which R&D does not include.

A shortcoming on the R&D approach is calculating the risk of inorganic contaminants. Inorganic chemicals do not react the way organics do in that they do not degrade and have half-lives.

Chapter 9

Conclusions and recommendations

The aim of Chapter 9 is to take together all the previous chapters, draw conclusions and make recommendations regarding the possible way forward for South Africa in addressing NAPL pollution.

In Chapter 2 the industries that may contribute towards organic pollution, apart from the heavy industries, were identified. Smaller scale urban activities that may contribute towards organic pollution were also identified and all these were plotted on a map of South Africa in order to determine the spatial distribution and density of industries. It was concluded that industries occur at a much higher frequency with a wider spatial distribution than may have been thought previously, i.e. industries are not only located at large metropolitan areas like Gauteng, Vereeniging, Durban and Port Elizabeth, but they also occur at places like Ermelo, Pietermaritzburg and Nelspruit.

In order to couple a risk to the industries, the type of organic variables that could be expected in association with industries, were identified and listed. The higher the number of associated organic chemicals, the higher risk the specific industry poses. This was used to rank the industries in terms of the risk they pose. The industries were overlain on Parsons' 1998 aquifer contamination susceptibility map and areas of concern were identified.

The following specific conclusions from Chapter 2 are highlighted below:

- Industries other than the petroleum refineries and steel works contribute towards organic pollution of aquifers (Section 2.1.4), which also need to be considered when drafting regulations pertaining to possible polluters. Small-scale industries like paint shops, auto-repair shops etc also contribute towards organic pollution (Section 2.1.6.4).

- Organic chemicals production in South Africa is dominated by the production of petroleum-related products (Section 2.1.5). The other five percent is made-up by the production of organic chemicals used in amongst others the cosmetics, pharmaceuticals and food industries.

- Approximately 5200 service stations may exist throughout South Africa that may cause pollution if the underground storage tanks leak (Section 2.1.6.1). Guidelines must be updated or drafted for the installation and monitoring of new underground storage tanks and for the remediation of leaking tanks.

- 16.3 million tons of industrial waste is generated per annum, the second highest contribution towards waste after mining. There are currently seven operating hazardous waste sites in South Africa that need to handle the waste generated by mostly industries. Several industries, however, have waste sites that accept only their own waste, and of all these industrial waste-sites only 30 are permitted (Section 2.1.6.2).

- Industries posing the highest risk are: Metal casting, structural metals manufacturing, fabricated metal manufacturing, tanning and dressing of leather, petrol refining, basic chemicals manufacturing and rubber and plastics manufacturing.

- The industry posing the least risk (smallest scale and covering the smallest area of South Africa), is the dressing and dyeing of fur. Chemical risk has been coupled with aquifer vulnerability to derive an associated industrial health risk.

In Chapter 3 the aim was to firstly understand the South African law and the implementation of the law, in order to be able to identify gaps in legislation that are measured in addressing NAPL pollution problems, as well as preventing pollution from occurring. The applicability of national legislation in terms of NAPLs has been highlighted. International conventions ratified by South Africa have also been overviewed and an assessment of the current implementation status has been made on these conventions. Currently only the Basil Convention is being included in the NEMA, while the other conventions still need some attention in the current legal system. A list of shortcomings in the legal system for addressing NAPL pollution was drawn up and the drafting of regulations is proposed for these shortcomings. A flow chart was also drawn up that highlights areas of concern (gaps), with proposed actions to be taken (for active sites and abandoned sites) and specific regulations that need to be drafted. For every action a responsible party has been designated (i.e. regulator, industry owner or consultant).

The following remarks are highlighted with respect to Chapter 3:

- Regulations must be updated to sufficiently address the problem of disposal, handling and storage of chemicals. Regulations can be the following:

  - Ensuring that diesel and petrol pollution occurrences are minimized on mining and industrial sites by requiring that the tanks *only* be installed above-ground, with a spillage capturing pit that can handle the volume of fuel kept in the tank, should the tank develop a leak.
  - Ensuring that areas where machinery and trucks of mines and industries receive fuel, are lined with a concrete slab and have a drainage system that can handle fuel spillage, where this waste water has to be disposed of at hazardous waste sites or treated.
  - Ensuring that (a) enough hazardous waste sites exist that (b) have the capacity to receive wastes and (c) can appropriately dispose of or treat the waste. Alternatively waste production can be minimized by requiring that industries and mines allocate part of their income, in association

with funding from government, to research and development of more environmentally friendly production processes. Similar regulations that require reduction of waste with the plan on rehabilitation cost savings can also be included in the mine closure plans for Environmental Management Programme Reports (EMPRs).

- Ensuring that trucks carrying waste to these waste sites are up to standard to handle the type of waste carried and ensuring that the drivers of these trucks know how to handle the possibility of a spillage (i.e. to report it to the local Fire Department and DWAF for immediate cleanup action).

- The hazardous waste sites will have to be upgraded or new ones located on suitable areas where underlying aquifers are not highly vulnerable, or waste generation will have to be reduced by incorporating recycling processes (e.g. re-use of waste water and using waste products as production material in other industrial processes).

- The problem of transport of chemicals (in the case of a road spillage) will have to be addressed.

- Interim procedures (protocols) for waste spillages (on road and at industries) need to be drafted and implemented, as well as emergency action plans for historical NAPL releases.

- Historical waste (dump) sites at abandoned sites need to be identified and the problem needs to be addressed.

- The different government departments need to streamline their processes in order to cut out unnecessary work, finish permitting procedures faster and prevent the illegal duplication of permitting disposal sites.

Chapter 4 was written in order to identify which parameters need to be measured in order to perform a site assessment and site characterization, with the ultimate goal of either remediation or risk assessment with the implementation of institutional management options. Only the most important physical parameters (NAPL and non-NAPL related) were identified and described, with the associated options available for analysis of these parameters. Appendix A is included on the CD, which list various VOCs and SVOCs with parameters identified for these variables.

Laboratories in South Africa were contacted in order to identify the analyses capabilities of these laboratories. It was concluded that South Africa does not have a large analysis capability, and that laboratories need to be upgraded. The laboratories can be upgraded to at least analyze for the “easy” parameters. Upgrading to a technologically advanced laboratory with specific analyses capabilities will cost South African laboratories a large amount of money and partial subsidy from government will be a great aid. Another option to explore is that a part of the money stored by industries and mines for future rehabilitation (according to the new Minerals Act) and be channeled into upgrading laboratories, after having identified gaps in analyses capabilities of the South African laboratories. This will also effect future cost savings when these entities have to rehabilitate and analyses capabilities have been established in South Africa, rather than to send samples overseas for analyses. Another costly exercise for laboratories is certification and accreditation. This is, however, a necessary expense for the quality assurance of detail environmental work. In Chapter 5 the lack of mobile laboratories was also identified and South African laboratories can explore the option of fitting vans with analyses equipment for field identification of variables, and hiring out these vans. This could save environmental investigators a lot of time while at the same time raising money for the laboratories.

In Chapter 5 site assessment has been described. Controversy exists over the existence and use of a site assessment phase before a site characterization phase. As can be seen from Chapter 5, site assessment could effect large cost-savings as it serves as a tool to form the initial conceptual model with. The site characterization phase will then serve as the conceptual model refinement phase.

The site assessment of each site will be specific and will depend on the characteristics of the site. As such, there is no fixed recipe to follow for performing a site assessment. Also, a must for each site, is the site visit. Conducting a desktop study only from the office could lead to missing pollution sources not mentioned in previous industry reports.

Most sites will require sampling and chemical analyses, but for some sites a few initial boreholes need to be drilled where at other sites existing boreholes that meet the sampling requirements can be used. The drilling of a few initial boreholes should not be seen as an unnecessary expenditure during site assessment since these boreholes give invaluable information needed for the site conceptual model, and on making decisions regarding extra boreholes, their placement and drilling them in such a manner as to prevent NAPL contamination spread.

The use of geophysics (if the site allows it) is recommended during site assessment since this could lead to cost-savings when drilling boreholes. Many new technologies exist by which NAPL pollution can be delineated in the subsurface (see Chapter 6, section 6.5). Some of these technologies, however, are in their development phase and results are not guaranteed. As such these technologies may incur larger costs for industries in developing countries like South Africa and should be applied with care. Depending on the site, it may be more cost-effective to drill a few more boreholes than to apply such a technology.

The use of rapid site assessment technologies may not be feasible in South Africa since these technologies are not readily available (to buy or to hire), which may lead to more expenditure rather than cost savings.

Chapter 6 focused specifically on site characterization methods. The applicability of different site characterization methods in unconsolidated formation versus hard rock was highlighted. In addition, the advantages and disadvantages of each method was highlighted, which may aid groundwater practitioners in identifying the applicable site characterization method(s) for the specific site under consideration. A short description was given of hard (fractured) rock in South Africa, with a description of the type of drilling methods that can be used in a hard rock environment. Drilling techniques that may be viable in the USA (core drilling) may not be economically viable in South Africa, due to costs involved. Also, the recovery rate of fracture zones with core drilling in comparison with air percussion is not much higher.

The following can be highlighted from Chapter 6:

- Several NAPL characteristics cause characterization difficulties and may compound characterization costs, which may include amongst others more expensive drilling techniques, safety precautions that need to be implemented during drilling, certain materials that need to be used during well-installation because of the corrosive nature of NAPL, certain sampling precautions that need be taken to ensure that volatile organics are not lost during sampling etc. Cost savings on some of the above-mentioned factors may lead to vital characterization and conceptual model mistakes, and is not recommended.

- Two types of characterization methods exist: Non-invasive and invasive. By first employing site-applicable non-invasive methods of characterization, one may lower the risk of possible wider NAPL contamination in the aquifer and this may also imply large cost-savings in that the choice and use of certain invasive methods may be more applicable to the site. This, in turn implies cost-savings on later re-characterizing the site due to poor choices made on characterization technologies that does not answer the questions that need to be answered. The non-invasive phase may be seen as a compulsory predecessor of the invasive characterization phase.

- An outside-in approach in terms of site characterization must always be followed in order to lower the possibility of spreading contamination during drilling and sampling programmes, especially in a hard rock environment.

- Geophysical techniques are becoming more useful as technologies advance and must be considered during site characterization since it would implicate large cost savings. See Section 6.5.

- It must first be determined if the site geology and suspected NAPL pollutant lends itself towards soil vapor analysis, before this type of analysis is performed, as can be seen in Section 6.5. If this analysis is performed indiscriminately, it may implicate money wasting since these surveys do not always yield useable information, if any. This technology is more applicable to LNAPL sites than to DNAPL sites.

- The effectiveness of different characterization methods must first be determined for a specific site before it is employed, since ineffective characterization methods could effect unnecessary expenditure.

In Chapter 7 a hypothetical case study is presented where the data presented in the previous chapters, are applied in order to perform a site assessment and characterization. The end purpose is to derive an impact rating for the presented site, which is obtained by performing an impact assessment. In performing an impact assessment, the impact that pollution from the site has on the surrounding region (in terms of water consumers and the environment) is described, where the rating assigned to the site describes the severity of the impact. This in turn can lead regulators to choosing the correct management options for the specific site, be they interim options, the planning for rehabilitation or institutional arrangements. The impact assessment is also an important predecessor for risk assessment, which is one management option that saves a lot of costs when considering rehabilitation.

The following problems associated with site assessment, site characterization and impact assessment exist, and need to be addressed by groundwater practitioners, the industry and regulators:

- The industry needs to keep better record of their actions on site, any building up or breaking down of works on-site, where contaminant materials are moved and stored. Such information is of cardinal importance when trying to assess the site and determine the impact that the site has on the surrounding environment. If the consultant does not know about chemicals that have been dumped in a small area previously and does not accidentally stumble upon it during the site assessment and characterization phases, this source of pollution can go undetected until it is picked up in the water much later and larger portions of the aquifer has already been contaminated. Pollution can especially go undetected in fractured rock environments with specific flow paths for certain pollutants. All the process wastes on-site must be identified by the industry and a final acceptable destination should be determined for each process waste. This was also highlighted in Chapter 2, where it was identified that less than five percent of all hazardous wastes reach hazardous waste disposal sites.

- Regulators should put regulations in place for manners in which to handle different industries and the wastes associated with each industry. Regionally, industries should be ranked in terms of their contribution towards organic pollution and the industries should be addressed according to their priorities.

- Groundwater practitioners should address problems such as determining apertures accurately in fractured rock environments since aperture sizes will govern the flow dynamics of NAPL and is one of the determining factors in fractured rock flow. The accurate determination of saturation should also be addressed. Much work still needs to be done in site characterization, in determining what the most cost effective ways are to perform site characterization, but that still answers the questions that need to be answered for risk assessment and site remediation.

  Before performing site characterization, the data needs should be determined by the consultant, as well as the means of obtaining this data. It would be incorrect to sample organic contaminants with disposable Teflon bailers just to save time on decontamination, if the disposable Teflon bailers will attribute significantly on the organic traces found in subsequent analysis of the sampled water. Similarly, the boreholes need to be cased correctly in order to be able to detect contaminants in the borehole. If the borehole is only cased up to a certain depth, NAPL may not be able to enter the well and although it is present in the aquifer, will not be picked up during the sampling run. If care is not taken to place the samples in the correct bottles (dark glass with Teflon caps) organic variables may degrade, volatilize or sorb onto the bottle, giving you a much lower concentration than what really is in the water.

These are just some of the considerations when performing site assessment and characterization on sites contaminated with organic pollutants.

In Chapter 8 risk assessment was performed on the same hypothetical site as was presented in Chapter 7. Different risk assessment programs were tested and compared in order to decide on the applicability of the different methods of risk assessment.

The following shortcomings were highlighted about risk assessment in general:

Certain uncertainties exist regarding risk assessment, which is encountered during different stages of risk assessment, such as:

- deficiencies in toxicity and dose-response data (shown in Section 8.6 above);
- deficiencies in data for contaminant behavior in soils and groundwater (e.g. koc values, half-lives);
- unknown, but probable, interacting toxic effects resulting from exposure to multiple toxicants;
- validity of the exposure model and other assumptions made in extrapolating from test animals to humans and from high to low doses;
- variations in the magnitude of toxic effect(s) expressed among and within different age groups of a population from exposure to a given toxicant;
- difficulties in estimating the duration and intensities of life-time exposure(s) to various toxicants.

Several generic datasets exist for values (i.e. foc values for certain types of soil, retardation factors for certain chemicals etc.), which could be used and referenced in risk assessments. Groundwater practitioners should, however, where possible, make measurements to obtain real data regarding a specific site in order to make the risk assessment conclusions as sound as possible. A sensitivity analyses on the risk assessment parameters is recommended for future research, to determine where costs can be saved with cutting field experiments on relatively insensitive parameters.

South African toxicologists should make available toxicity standards for all missing / incomplete organic and inorganic constituents after taking into account all tests conducted up to date on animals and plants.

A comparison between the different risk assessment methods:

On a comparison between risk assessment using the R&D approach and RISC Workbench, the following conclusions can be made:

- RISC Workbench and the R&D approach identified the same chemicals as chemicals of concern, but RISC Workbench identified more chemicals than R&D. It would seem that RISC Workbench is more conservative in its approach. Both methods use a groundwater model and the source-pathway-receptor principle, with the difference that in R&D, the values have to be entered into the program. Choosing "incorrect" values from literature may result in an over- or under estimation of the associated risk. A thorough literature check and the choosing of variables that showed repeatability during laboratory testing, is advised

- The values for receptor well concentrations of the R&D and the RISC Workbench assessments differ, with the receptor well concentrations consistently lower for RISC Workbench than for R&D. In this respect it seems that the R&D assessment tool is more conservative than RISC Workbench.

To aid the R&D risk assessment, a dose response analyses was performed on the data, and chloroform, m-xylene, benzene, tetrachlorethene and phenol was identified as chemicals of concern. Napthalene, phenanthrene and anthracene was also highlighted, but these are rather immobile since they sorb strongly onto soil particles, and the associated risk was thus lowered. A good correlation exist between the *toxicity assessment* and the *exposure assessments* (R&D, RISC Workbench), but since these two approaches are entirely different tools, the toxicity assessment should not be used to replace an exposure assessment, but should be used in conjunction with exposure assessments, if the exposure assessment tool does not include a toxicity assessment.

Urban risk assessment was also performed and the following conclusions can be made regarding the Urban risk assessment tool:

- The R&D, RISC Workbench and Urban risk assessment all highlighted the most important contaminants of concern and showed relatively the same risk.

- The program is a good first screening tool of the most highly expected contaminants. This program will therefore give a manager a good idea of what contaminants to expect in association with a certain industrial process.

- The program does not make use of the source-pathway-receptor principle when calculating risk, which the R&D method and the RISC Workbench do take into account when calculating the risk of a certain chemical. In this respect, the urban risk assessment program may over-estimate risk and be too conservative in comparison with the R&D approach and the RISC Workbench program.

- The Tier 2 risk percentages were constantly lower than the Tier 1 values. The screening level risk was lower than Tier 1 and 2, and may be due to the fact that site-specific values are not taken into account. The screening level risk (Tier 0) may thus be lower or higher than the site-specific tier 1 and 2 risk percentages.

The risk assessment programs were compared to derive the best program to use for risk assessment. It was concluded that if you want a screening level answer and are a typical manager that has to make a decision on a starting point for addressing a polluted site, the Urban Risk Assessment program would be the best tool to use. Typical questions that can be answered are: *What contaminants must be analyzed for associated with a certain industrial activity? What contaminants pose the highest health risk?* This program also specifically addresses risk in urban environments and have taken into account contaminants typically associated with certain sources in an urban environment. This is not an in-depth risk assessment tool and if the need is risk assessment on which decisions such as risk minimization measures and determination of the need of remediation or determination of remedial targets must be made, a program such as RISC Workbench must be used. This program takes into account the source, pathway and receptor (as does the R&D method), which is necessary when determining the real risk associated with a contamination source situated 100 m away from a receptor, as opposed to being 50 m away from a receptor. In this respect the URA may over-estimate the risk associated with certain chemicals.

The R&D approach is similar to RISC Workbench in that you can determine receptor well concentrations (given certain source concentrations) of a contaminant, as well as the cleanup levels. The R&D approach has limitations in that the target concentrations and half-lives of the chemicals must be carefully chosen. The Kd values must be determined from measured *foc* values in order to calculate representative and accurate contaminant retardation factors. None of the solutions presented by the R&D methodology may be applicable to a highly heterogeneous aquifer (a highly fractured aquifer for example). RISC Workbench also has built in hazard and toxicity assessments, which R&D does not include. A shortcoming on the R&D approach is calculating the risk of inorganic contaminants. Inorganic chemicals do not react the way organics do in that they do not degrade and have half-lives and more research is suggested for determining the risk of inorganic contaminants.

In conclusion it was identified that South Africa still needs to do a lot of work to get up to speed with international practice. South Africa should learn from mistakes other countries have made and should use methods applicable to South African conditions, which does not necessarily mean copying all international work, as could be seen from the use of core drilling versus air percussion. In terms of the large amount of hard rock present in South Africa, the country poses particular challenges, which have to be addressed as the knowledge base related to organic studies in South Africa increase.

Chapter 10

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APPENDIX A

NAPL PHYSICAL PARAMETERS

APPENDIX A

DATA SET 1 – VOC’s

Name	Type of chemical substance	Ref	Molc weight	Ref	Solubility in water mg/L	@ T	Ref	Koc (mL/g)	Alternative Koc (mL/g)	Ref	Log Koc (mL/g)	Ref	Molc structure	Ref
Acetone			58.08	2	1000000		2	0.575		2				
Benzene	aromatic	8	78.11	3	1780, 1780	25	5,3	87.78089408	61.7	8,2	1.9434	Est from Kow	C6H6	7
Bromobenzene			157.01	1	500	20	1	213.796209		1	2.33	1	C6H5Br	1
Bromochloromethane			129.39	1	16700	20	1	26.91534804		1	1.43	1	CH2-Br-Cl	7
Bromodichloromethane			163.83	1	4500	20	1	61.65950019		1	1.79	1	CHBrCl2	7
Bromoform	chlrnd alkane	8	252.73	1	3010	20	1	281.8382931		1	2.45	1	CHBr3	1
Bromomethane			94.9387	4	51220		4	19.39545624		5	1.2877	Est from Kow	C-H3-Br	7
Carbon disulfide			76.14	2	1190		2	45.7		2				
Carbon tetrachloride	chlrnd alkane	8	153.28	1	800	20	5	436.5158322		1	2.64	1	CCl4	7
Chlorobenzene	chlrnd aromatic	8	112.56	1	490, 500	25	5,1	47.86300923		1	1.68	1	C6-H5-Cl	7
Chloroethane			64.5	2	5740		2	143		2				
Chloroform	chlrnd alkane	8	119.38	1	8000	20	1	43.65158322		1	1.64	1	CH-Cl3	7
cis-1,2-Dichloroethene			96.9438	4	8000		4						C2-H2-Cl2	7
Dibromochloromethane			208.28	1	4000	20	1	83.17637711		1	1.92	1	CHBr2Cl	7
Dibromomethane			173.8348	4	11930		4						C-H2-Br2	7
Dichlorodifluoromethane	chlrnd alkane	8	120.9138	4	280	25	4	110.9685727		8	2.0452	Est from Kow	C-Cl2-F2	7
Dichloromethane			84.9328	4	13200		4	198		14			C-H2-Cl2	7
Ethylbenzene	aromatic	8	106.17	3	150, 160, 150	25	5,3	821.2965528		8	2.9145	Est from Kow	C8H10	
Ethylether			74.1	2				73		2				
Formaldehyde			30.03	2	400000		2	NA		2				
Formic acid			46.2	2	1000000		2	NA		2				
n-Hexane			86.2	2	9.5		2	890		2				
Hexachlorobutadiene	chlrnd alkane	8	260.76	1	2.55		1	4677.351413		1	3.67	1	C4Cl6	1
Isobutyl-alcohol			74.12	2	55000		2	60		2				
Isopropylbenzene			120.1938	4	49.9		4							
m,p-Xylene					160-180, 200a	25	5	775.5324958		2	2.8896	6	C8H10	
Naphthalene	aromatic	8	128.6	3	31.7, 32		5,3	21.75204034		8	1.3375	Est from Kow	C10H8	
n-Butylbenzene			134.2206	4	insoluble, 11.8		4,2	2.46	3523.0759	14,2			C10H14	4
n-propylbenzene			120.1938	4	insoluble, 23.4		4,2	2176.707131	725	1,2	3.3378	Est from Kow	C9H12	4
o-Xylene			106.167	4	insoluble, 170a, 170		4,5,2	2.40E+02		18			C8H10	
sec-Butylbenzene			134.2206	4	17.6		2	4981.76228		2			C10H14	4
Styrene (Vinyl benz.)			104.1512	4	320		4	549.7940051		5	2.7402	Est from Kow	C8H8	4
tert-Butylbenzene			134.2206	4	29.5		2	2153.322112		2			C10H14	4
Tetrachloroethene			165.83	1	150	20	1	263.0267992		1	2.42	1	CCl2=CCl2	
Toluene	aromatic	8	92.1	3	500, 500		5,3	340.9573053		8	2.5327	Est from Kow	C7H8	
trans-1,2-Dichloroethene			96.94	1	400	20	1	58.88436554		1	1.77	1	C2-H2-C12	7
Trichloroethene			131.39	1	1100, 1.1	20	1,2	125.8925412		1	2.1	1	C3HCl3	7

Name	Type of chemical substance	Ref	Molc weight	Ref	Solubility in water mg/L	@ T	Ref	Koc (mL/g)	Alternative Koc (mL/g)	Ref	Log Koc (mL/g)	Ref	Molc structure	Ref
Trichlorofluoromethane* (1,1,2 Tri…)	chlrnd alkane	3	137.37	1	1100	20	1	158.4893192		1	2.2	1	C-C13-F	7
Vinyl chloride	chlrnd alkane	8	62.4987	4	1100, 1.1	25	4,3	20.93630324		8	1.3209	Est from Kow	C2-H3-Cl	7
1,1,1,2-Tetrachloroethane			167.8498	4	<1000, 1100	20.5	4,2	399		2			C2-H2-Cl4	7
1,1,1-Trichloroethane	chlrnd alkane	8	133.4	1	4400, 1.36e+3	20	5,1,2	151.3561248	135	1,2	2.18	1	C2H3Cl3	7
1,1,2,2-Tetrachloroethane	chlrnd alkane	8	167.85	1	2900	20	1	117.4897555	79	1,2	2.07	1	C2H2Cl4	
1,1,2-Trichloroethane	chlrnd alkane	8	133.4	1	4500	20	1	56.23413252	75	1,2	1.75	1	C2H3Cl3	7
1,1-Dichloroethane	chlrnd alkane	8	98.96	1	5500	20	1	30.1995172		1	1.48	1	C2-H4-C12	7
1,1-Dichloroethene			96.94	1	400	20	1	15.13561248	65	1,2	1.18	1	C2-H2-C12	7
1,1-Dichloropropene			110.9706	4									C3-H4-Cl2	7
1,2,3-Trichlorobenzene			181.4487	4	insoluble		4						C6H3C13	7
1,2,3-Trichloropropane			147.43	1	1800		4	181.4679779		5	2.2588	Est from Kow	C3H5Cl3	1
1,2,4-Trichlorobenzene	chlrnd aromatic	8	181.45	1	19	20	1	9549.92586		1	3.98	1	C6H3C13	1
1,2,4-Trimethylbenzene			120.1938	4	Slightly soluble		4	2735.268726		5	3.437	Est from Kow	C9H12	4
1,2-Dibromo-3-chloropropane			236.3335	4	1230		4	129		14			C3H5Br2 Cl	4
1,2-Dibromoethane			187.8616	4	4152		4	44		14			C2-H4-Br2	7
1,2-Dichlorobenzene (o)	chlrnd aromatic	8	147	1	83.96, 100	20	4,1	186.2087137	1789101	1,2	2.27	1	C6H4Cl2	1
1,2-Dichloroethane	chlrnd alkane	8	98.96	1	8700, 5500	20	5,1	30.1995172		1	1.48	1	C2H4C12	7
1,2-Dichloroethene (cis)			96.94	2	3500		2	35.5		2				
1,2-Dichloropropane	chlrnd alkane	8	112.9	1	2700		1	51.2861384		1	1.71	1	C3H6Cl2	7
1,3,5-Trimethylbenzene			120.1938	4	insoluble		4						C9H12	4
1,3-Dichlorobenzene (m)	chlrnd aromatic	8	147	1	111	20	1	169.8243652	300	1,2	2.23	1	C6H4Cl2	1
1,3-Dichloropropane			112.9864	4	insoluble		4						C3-H6-Cl2	7
1,3-Dichloropropene			110.98	2	2800		2	21.7		2				
1,4-Dichlorobenzene (p)	chlrnd aromatic	8	147.0036	4	81.3		4	1299.271763	616	8,2	3.1137	Est from Kow	C6H4Cl2	4
1,4-Dioxane			88.1	2	1000000		2	17		2				
2,2-Dichloropropane			112.9864	4									C3-H6-Cl2	7
2-Chlorotoluene (o-")			126.5853	4	72	20	1	1584.893192		1	3.2	1	C7H7Cl	4
4-Chlorotoluene (p-Chlorotoluene)			126.59	1	44	20	1	1202.264435		1	3.08	1	C7H7Cl	1
4-Isopropyltoluene			134.2206	4	insoluble		4						C10H14	4

Name	CAS No	Ref	Boiling Point	Ref	Flash Point degr celc	Ref	Spc. Density (gm/cm3) / (g/cc)	@ T	Ref	Absolute Viscosity	Ref	Vapor P mmHg	@ T	Ref
Acetone	67-64-1	2												
Benzene	71-43-2	7	80.1	5			0.88		5	0.604	5	47.8	10	5
Bromobenzene	108-86-1	1	156	1	51	1	1.495		1	0.99	1	3.3		1
Bromochloromethane	74-97-5	7	68	1	NC	1	1.934		1	0.57	1	1.41		1
Bromodichloromethane	75-27-4	7	90	1			1.98		1	1.71	1	50		1
Bromoform	75-25-2	1	149	1	NC	1	2.89		1	2.02	1	4		1
Bromomethane	74-83-9	7	3.56	4			1.732		4					
Carbon disulfide	75-15-0	2												
Carbon tetrachloride	56-23-5	7	76.8, 77	5,1	NC	1	1.5833, 1.594	25	5,1	0.908, 0.97	5,1	58.3, 9e+	10	5,1
Chlorobenzene	108-90-7	7	131.7, 13	5,1	28	1	1.1007, 1.106	25	5,1	0.753, 0.8	5,1	6.9, 9, 8.8	10	5,1,4
Chloroethane	75-00-3	2												
Chloroform	67-6-3	7	62	1	NC	1	1.483		1	0.58	1	160		1
cis-1,2-Dichloroethene	156-59-2	7	60	4	6	4	1.284		4					
Dibromochloromethane	124-48-1	7	117	1			2.451		1			76		1
Dibromomethane	74-95-3	7	97	4			2.497		4					
Dichlorodifluoromethane	75-71-8	7	-29.79	4			1.329		4	0.0117 cP	9			
Dichloromethane	75-09-2	7	39.8	4			1.3255		4			350		4
Ethylbenzene	100-41-4	7	136.2	5			0.8654	25	5	0.631	5	6	10	5
Ethylether	60-29-7	2												
Formaldehyde	50-00-0	2												
Formic acid	64-18-6	2												
n-Hexane	110-54-3	2												
Hexachlorobutadiene	87-68-3	1	215	1	NC	1	1.554		1	2.45	1	0.15		1
Isobutyl-alcohol	78-83-1	2												
Isopropylbenzene			151	4	31	4	0.862		4			3.5		4
m,p-Xylene			138.4-14	5			0.857-0.876	25	5	0.608-0.80	5, 11, 11	4.5-5.6	10	5
Naphthalene	91-20-3	4	218	4	78	4	0.997		4	0.45	8	4.42		4
n-Butylbenzene	104-51-8	4	183	4	59	4	0.86		4					
n-propylbenzene	103-65-1	4	159	4	47	4	0.862		4					
o-Xylene	95-47-6	7	144	4	32	4	0.897		4	0.802a	11	5.2		4
sec-Butylbenzene	135-98-8	4	173	4	45	4	0.862		4					
Styrene (Vinyl benz.)	100-42-5	4	145.2	4	32	4	0.9045		4	0.751a	11	5		4
tert-Butylbenzene	98-06-6	4	169	4			0.867		4					
Tetrachloroethene	127-18-4	7	121, 121	1,3			1.623, 1.62		1,3	0.89	1	14		1
Toluene	108-88-3	7					0.867		8	0.522	8	10		8
trans-1,2-Dichloroethene	157-60-5	7	47	1	2	1	1.257		1	0.4	1	265	20	1
Trichloroethene	79-01-6	7	87	1	32.2	1	1.464		1	0.57	1	57.8		1

Name	CAS No	Ref	Boiling Point	Ref	Flash Point degr celc	Ref	Spc. Density (gm/cm3) / (g/cc)	@ T	Ref	Absolute Viscosity	Ref	Vapor P mmHg	@ T	Ref
Trichlorofluoromethane* (1,1,2 Tri…	75-69-4	7	24	1	NC	1	1.487		1	0.42	1	687	20	1
Vinyl chloride	75-01-4	7	-13.9	4	42	4	0.9106		4					
1,1,1,2-Tetrachloroethane	630-20-6	7	130.5	4			1.5532		4					
1,1,1-Trichloroethane	71-55-6	7	74.1, 74,	5,1,3	NC	1	1.33, 1.35		5,3	0.793, 1.2	5,1	67.4, 1e+	10, 20	5,5
1,1,2,2-Tetrachloroethane	79-34-5		146	1	NC	1	1.595, 1.60		1,3	1.75	1	5		1
1,1,2-Trichloroethane	79-00-5	7	114, 113	1,3			1.44, 1.43		1,3	0.12	1	19		1
1,1-Dichloroethane	75-34-3	7	57.4, 56	5	-6	1	1.17, 1.235, 1.18		5,1,3	0.464, 0.8	5,1	125.8, 182	10	5,1
1,1-Dichloroethene	75-35-4	7	37, 31.9	1,3	-15	1	1.218		3			495		1
1,1-Dichloropropene	563-58-6	7												
1,2,3-Trichlorobenzene	87-61-6	7	219	4	126	4	1.69		4					
1,2,3-Trichloropropane	96-18-4	1	142	1	73.3	1	1.3889		1			2		1
1,2,4-Trichlorobenzene	120-82-1	1	210	1	105	1	1.4		1	1.42	1	0.4		1
1,2,4-Trimethylbenzene	95-63-6	4	169	4	48	4	0.876		4					
1,2-Dibromo-3-chloropropane	96-12-8	4	195	4			2.05		4					
1,2-Dibromoethane	106-93-4	7	131.7	4	1	4	2.17		4					
1,2-Dichlorobenzene (o)	95-50-1	1	180	1	67	4	1.305		1	1.32	1	1		1
1,2-Dichloroethane	75-34-3	7	57.4, 56	5,1	13	1	1.257, 1.176, 1.23		5,1,3	0.779, 0.44	5,1	40, 1.82e-	10, 20	1
1,2-Dichloroethene (cis)	156-59-2	2												
1,2-Dichloropropane	78-87-5	7	96	1	15.6	1	1.56		5	0.86	1	42		1
1,3,5-Trimethylbenzene	108-67-8	4	165	4	44	4	0.865		4			1.86		4
1,3-Dichlorobenzene (m)	541-73-1	1	173	1	63	1	1.288		1	1.04	1	2.3		1
1,3-Dichloropropane	142-28-9	7	120.4	4	20	4								
1,3-Dichloropropene	542-75-6	2												
1,4-Dichlorobenzene (p)	106-46-7	4	173.4	4	67	4	1.2417		4			0.4		4
1,4-Dioxane	123-91-1	2												
2,2-Dichloropropane	549-20-7	7	69	4			1.112		4					
2-Chlorotoluene (o-")	95-49-8, 95	4,1	158.97	4	47	4	1.082		4	0.75	1	2.7		1
4-Chlorotoluene (p-Chlorotoluen	106-43-4	1	162	1			1.066		1			4.5		1
4-Isopropyltoluene	99-87-6	4	176 - 178	4	47	4	0.86		4					

Name	Henry's Law Cnst. (atm-m3/mol)	Ref	log Kow (L)	Ref	Diff coeff in H2O (sq.cm/sec)	Ref	Heat of Vaporization	Ref	Surface tension	Ref	Interfacial tension	Ref	Kd determinable: Koc*foc
Acetone			-0.24	2									1
Benzene	0.22	5	1.98	8	0.0000098	2	33.83	5					1
Bromobenzene	0.0024	1	3.01	1					35.8	1	39.8	1	1
Bromochloromethane	0.00144	1	1.41	1					33.3	1			1
Bromodichloromethane	0.000212	1	1.88	1									1
Bromoform	0.000532	1	2.3	1					45.5	1			1
Bromomethane	*532*	12	1.19	13									1
Carbon disulfide	0.0303	2	2	2	0.00001	2							1
Carbon tetrachloride	0.807, 3.02e-2	5,1	2.83	1	0.0000088	2	32.43	5	27	1	45	1	1
Chlorobenzene	0.14*, 4.45e-3	5,1	2.84	1	0.0000079	1	40.97	5	33.2	1	37.4	1	1
Chloroethane	0.00848	2	1.92	2	0.0000153	2							1
Chloroform	0.0032	1	1.95	1	0.0000091	1			27.2	1	32.8	1	1
cis-1,2-Dichloroethene	*299, 460*	12											0
Dibromochloromethane	0.00099	1	2.08	1	0.0000105	2							1
Dibromomethane													0
Dichlorodifluoromethane	*26, 40.6*	12	2.16	8	0.00001	2							1
Dichloromethane	*173, 301*	12	1.25	12									1
Ethylbenzene	0.323	5	3.15	8	0.0000078	2	42.24	5					1
Ethylether	0.00123	2											1
Formaldehyde	0.000000337	2			0.0000174	2							0
Formic acid	0.000000167	2			0.0000171	2							0
n-Hexane	1.81	2			0.00000816	2							1
Hexachlorobutadiene	0.026	1	4.78	1									1
Isobutyl-alcohol													1
Isopropylbenzene													0
m,p-Xylene	0.20, 0.214, 6.91e-3, 7.01	5,11	3.12	6	0.00000846	2	42.4-43.43	5					1
Naphthalene	0.0025	8	1.25	8									1
n-Butylbenzene			4.29	12	0.00000734	2							1
n-propylbenzene	*893, 1090*	12	3.66	12	0.00000783	2							1
o-Xylene	0.00494a	11			0.00000846	2							0
sec-Butylbenzene	0.0176	2			0.00000734	2							1
Styrene (Vinyl benz.)	2.28e-3a	11	2.94	12									1
tert-Butylbenzene	0.0132	2			0.00000738	2							1
Tetrachloroethene	0.0153	1	2.6	1	0.0000075	1			31.3	1	44.4	1	1
Toluene	0.0057	8	2.69	8									1
trans-1,2-Dichloroethene	0.384	1	2.09	1	0.0000095	1			25	1	30	1	1
Trichloroethene	0.0091	1	2.53	1	0.0000083	1			29.3	1	34.5	1	1

Name	Henry's Law Cnst. (atm-m3/mol)	Ref	log Kow (L)	Ref	Diff coeff in H2O (sq.cm/sec)	Ref	Heat of Vaporization	Ref	Surface tension	Ref	Interfacial tension	Ref	Kd determinable: Koc*foc
Trichlorofluoromethane* (1,1,2 Tri…)	0.11	1	2.53	1					29.3	1	34.5		1
Vinyl chloride			1.23	8									1
1,1,1,2-Tetrachloroethane	0.00242	2	2.93	2	0.0000093	2							1
1,1,1-Trichloroethane	1.13, 1.8e-2, 1.72e-02	5,1,2	2.47	1	0.000008	1			25.4	1	45	1	1
1,1,2,2-Tetrachloroethane	0.00038, 3.45E-4	1,2	2.56	1	0.0000079	2			36	1			1
1,1,2-Trichloroethane	0.00074, 9.13E-04	1,2	2.18	1	0.000008	1			34	1			1
1,1-Dichloroethane	0.234, 0.0043	5,1	1.78	1			30.62	5	24.8	1			1
1,1-Dichloroethene	0.021	1	2.13	1	0.0000095	1			24	1	37	1	1
1,1-Dichloropropene													0
1,2,3-Trichlorobenzene													0
1,2,3-Trichloropropane	0.000318	1	2.36	12									1
1,2,4-Trichlorobenzene	0.00232	1	4.02	1					39.1	1			1
1,2,4-Trimethylbenzene			3.78	12									1
1,2-Dibromo-3-chloropropane			2.26	12									1
1,2-Dibromoethane	61.8	12	1.6	12									1
1,2-Dichlorobenzene (o)	0.0019	1	3.4	1	0.0000079	2	61.51	5	37	1	40	1	1
1,2-Dichloroethane	0.04, 4.3e-3	5,1	1.78	1			35.61	5	24.8	1			1
1,2-Dichloroethene (cis)	0.00408	2	1.86	2	0.0000113	2							1
1,2-Dichloropropane	0.0023	1	2.28	1					28.7	1			1
1,3,5-Trimethylbenzene													0
1,3-Dichlorobenzene (m)	0.0036, 2.83E-03	1,2	3.38	1	0.00000885	2			33.2	1			1
1,3-Dichloropropane													0
1,3-Dichloropropene	0.0177	2	2	2	0.00001	2							1
1,4-Dichlorobenzene (p)	149, 262, 0.00243	12,2	3.39	8	0.0000079	2							1
1,4-Dioxane	0.0000048	2	-0.27	2	0.0000105	2							1
2,2-Dichloropropane													0
2-Chlorotoluene (o-")	0.00625	1	3.42	1					32.9	1			1
4-Chlorotoluene (p-Chlorotoluene)	0.017	1	3.3	1					34.6	1			1
4-Isopropyltoluene													0

Name	Kd gravel	Ref	Kd sand fine	foc	Ref	Kd Silt	foc	Ref	Half life soil (days)	Ref	Half life GW (days)	Ref
Acetone												
Benzene			0.079	0.00023	16	0.092	0.0018	16	8.6-248	8	10-730	58
Bromobenzene												
Bromochloromethane												
Bromodichloromethane												
Bromoform									28-180	1	56-360	1
Bromomethane												
Carbon disulfide												
Carbon tetrachloride			1.8 to 2.5		4				180-360	1	7-360	1
Chlorobenzene	33	15	33		15	33		15	68-150	1	136-300	1
Chloroethane												
Chloroform	2.5-3.8	15	2.5-3.8		15	2.5-3.8		15	28-180	1	56-1800	1
cis-1,2-Dichloroethene												
Dibromochloromethane	6	15	6		15	6		15	28-180	1	14-180	1
Dibromomethane												
Dichlorodifluoromethane												
Dichloromethane												
Ethylbenzene									126	8		
Ethylether												
Formaldehyde												
Formic acid												
n-Hexane												
Hexachlorobutadiene									28-181	1	56-361	1
Isobutyl-alcohol												
Isopropylbenzene												
m,p-Xylene			0.119, 0.383, 0.261	0.00017, 0.00023, 0.00028	16	0.569	0.00108	16	long	8	long	8
Naphthalene											3	59
n-Butylbenzene												
n-propylbenzene												
o-Xylene									126	8	1.2-31	8
sec-Butylbenzene												
Styrene (Vinyl benz.)												
tert-Butylbenzene												
Tetrachloroethene			2.7-5.9		4				180-360	1	360-720	1
Toluene			0.072	0.00026	16	0.199	0.00108	16	126	8		
trans-1,2-Dichloroethene												
Trichloroethene	2.14								180-360	1	321-1653	1

Name	Kd gravel	Ref	Kd sand fine	foc	Ref	Kd Silt	foc	Ref	Half life soil (days)	Ref	Half life GW (days)	Ref
Trichlorofluoromethane* (1,1,2 Tri…)									180-360	1	360-720	1
Vinyl chloride												
1,1,1,2-Tetrachloroethane												
1,1,1-Trichloroethane									140-273	1	140-546	1
1,1,2,2-Tetrachloroethane									0.45-45	1	0.45-45	1
1,1,2-Trichloroethane									136-720	1	136-720	1
1,1-Dichloroethane									32-154	1	64-154	1
1,1-Dichloroethene									28-180	1	56-132	1
1,1-Dichloropropene												
1,2,3-Trichlorobenzene												
1,2,3-Trichloropropane									180-360	1	360-720	1
1,2,4-Trichlorobenzene									28-180	1	56-360	1
1,2,4-Trimethylbenzene												
1,2-Dibromo-3-chloropropane												
1,2-Dibromoethane												
1,2-Dichlorobenzene (o)									28-180	1	56-360	1
1,2-Dichloroethane									100-180	1	100-360	1
1,2-Dichloroethene (cis)												
1,2-Dichloropropane									167-1289	1	334-2592	1
1,3,5-Trimethylbenzene												
1,3-Dichlorobenzene (m)									28-180	1	56-360	1
1,3-Dichloropropane												
1,3-Dichloropropene												
1,4-Dichlorobenzene (p)												
1,4-Dioxane												
2,2-Dichloropropane												
2-Chlorotoluene (o-")												
4-Chlorotoluene (p-Chlorotoluene)												
4-Isopropyltoluene												

Name	Usage	Ref
Acetone	Intermediate-manufacture industrial solvents; direct uses in plastics	17
Benzene	Detergents, intermediate, solvents, gasoline, coal tar by-product	3
Bromobenzene	solvent, motor oils, organic synthesis	3
Bromochloromethane	Used in fire extinguisher fluid, intermediate and solvent for manufacture pesticides	19
Bromodichloromethane	Solvent, fire extinguisher fluid, mineral and salt seperations	3
Bromoform	Solvent, intermediate	3
Bromomethane	soil fumigation, quarantine and commodity fumigation, chemical intermediates	20
Carbon disulfide	Solvent, chem Intermed for rubber compounds, fumigant: commodities, catalyst, cold vulcunization of rubber	21
Carbon tetrachloride	degreasers, refrigerants, propellants, fumigants, chemical manufacturing	3
Chlorobenzene	solvent, pesticides, chemical manufacturing	3
Chloroethane	Blowing agent: foamed plastics, previous uses: production tetraethyl lead in leaded gasoline	22
Chloroform	plastics, fumigants, insecticides, refrigerants, propellants	3
cis-1,2-Dichloroethene	Solvent, chemical intermediate for perfumes, dyes, lacquers, rubber; manufacture of pharmaceuticals	23
Dibromochloromethane	organic synthesis	3
Dibromomethane	Organic synthesis, solvent	3
Dichlorodifluoromethane	Blowing agent for polymers, foaming agent in fire extinguishers, water purification, petroleum recovery, regulating device leak detection, used in organic synthesis: freons	24
Dichloromethane	In paint strippers, aerosols, solvent, cleaner in chemical processing, urethane blowing agent, metal degreasing, fumigant, pharmaceuticals - anesthetic	25
Ethylbenzene	Intermediate, solvent, gasoline, coal tar by-product	3
Ethylether	Pharmaceutical, Extraction solvent, organic synthesis, laboratory reagents	26
Formaldehyde	Disinfectant, germicide, chemical intermediate,	27
Formic acid	Preservative,antibact agent:livestock feed, poultry:kill salmonella, leather-tannery agent	28
n-Hexane	Production of solvents, cleaning agents, vegetable oil extractor	29
Hexachlorobutadiene	solvent, transformer and hydraulic fluid, heat transfer liquid	3
Isobutyl-alcohol	Solvent in paints & lacquers, manufacture of isobutyl esters	30
Isopropylbenzene	Principal chemical for production of phenol.Starting material for acetophenone, a-methylstyrene. Minor uses: as a thinner; raw material for peroxides and oxidation catalysts and solvent for fats and resins.	31
m,p-Xylene	Aviation gasoline protective coatings, solvent, synthesis of organic chemicals, gasoline, coal tar by-product	3
Naphthalene	solvent, lubricant, explosives, preservatives, intermediate, fungicide, moth repellant, coal tar by-product, gasoline	3
n-Butylbenzene	Intermediate of synthesis of chemicals and raw material for liquid crystal	32
n-propylbenzene	dyestuffs, solvent	3
o-Xylene	Aviation gasoline protective coatings, solvent, synthesis of organic chemicals, gasoline, coal tar by-product	3
sec-Butylbenzene		
Styrene (Vinyl benz.)	Plastics, resins, protective coatings, intermediate, gasoline	3
tert-Butylbenzene	used as the raw materials for bulclizine, convallaria aldehyde	33
Tetrachloroethene	Used in dry cleaning as industrial solvent, metal-degreasing. Starting material (building block) and used in some consumer products.	34
Toluene	Adhesive solvent in plastics, solvent, aviation and high-octane blending stock, dilutent and thinner, chemicals, explosives, detergents, gasoline, coal tar by-product	3
trans-1,2-Dichloroethene	Intermediate in the manufacture of other products	35
Trichloroethene	Solvent to remove grease from metal parts, can also be found in some household products, including typewriter correction fluid, paint removers, adhesives, and spot removers	36

Name	Usage	Ref
Trichlorofluoromethane* (1,1,2	Solvent, blowing agent: polyurethane foams, dry cleaning agent, aerosol propellant, in fire extinguishers. Manufacturing: commercial refrigeration equipment & cleaning compounds	37
Vinyl chloride	Make poly vinyl chloride (PVC), in furniture / automobile upholstery, refrigerant	38
1,1,1,2-Tetrachloroethane	Intermediate for producing tri- and tetra- chloroethylene	39
1,1,1-Trichloroethane	Solvent to dissolve glue and paint, removes oil or grease from manufactured metal parts. Found in spot cleaners, glues, and aerosol sprays.	40
1,1,2,2-Tetrachloroethane	Produce trichloroethylene, tetrachloroethylene. Solvent, metal degreaser, in paint removers, varnishes lacquers, photographic films and in pesticides, oils and fats extractant.	41
1,1,2-Trichloroethane	Chemical intermediate for 1,1-dichloroethene. Solvent for chlorinated rubbers, fats, oils, waxes, and resins.	42
1,1-Dichloroethane	Intermediate for vinyl chloride, 1,1,1-trichloroethane, high vacuum rubber, solvent for plastics, oils, and fats (limited), past used as anesthetic.	43
1,1-Dichloroethene	Intermediate, production of polyvinylidene chloride copolymers, used as films for food packaging, carpet backing and in piping, coating for steel pipes.	44
1,1-Dichloropropene		
1,2,3-Trichlorobenzene	Process solvent, parent compound in synthesis of pesticides (mainly), plastics, dyes, pharmaceuticals. Insecticidal fumigants, draincleaners.	45
1,2,3-Trichloropropane	Intermediate, industrial solvent, paint and varnish remover, cleaning and degreasing agent.	46
1,2,4-Trichlorobenzene	Intermediate for herbicides, used as solvent, dielectric fluid, degreaser and lubricant.	47
1,2,4-Trimethylbenzene	Manufacture of dyestuffs, pharmaceuticals, chemical manufacturing, gasoline	3
1,2-Dibromo-3-chloropropa	Used as soil fumigant and nematocide (now suspended), intermediate for synthesis of organics.	48
1,2-Dibromoethane	Used as soil pesticide (suspended), log treatment for termites, dye and wax preparation.	49
1,2-Dichlorobenzene (o)	Solvent , insecticide, intermed in mfr of dyes; degreaser for metals, leather, wool, Herbicide, insecticide, soil fumigant, magnetic coil coolant; wood preserving, intermediate agric chemicals	50
1,2-Dichloroethane	Solvent, degreasers, soaps and scouring compounds, organic synthesis, addative in antiknock gasoline, paint and finish removers	3
1,2-Dichloroethene (cis)	Used to produce solvents and in chemical mixtures	51
1,2-Dichloropropane	Solvent, intermediate, scouring compounds, fumigant, nematocide, addative for antiknock fluids	3
1,3,5-Trimethylbenzene		
1,3-Dichlorobenzene (m)	Solvent, chemical intermediate to manufacture dyes, agrochemicals, pharmaceuticals and other organics. Insecticide and a fumigant.	52
1,3-Dichloropropane	Soil fumigant	54
1,3-Dichloropropene	Soil fumigant for the control of nematodes in vegetables, potatoes, and tobacco.	53
1,4-Dichlorobenzene (p)	Control moths, molds, and mildew, and to deodorize restrooms and waste containers	55
1,4-Dioxane	Solvent for cellulose, resins, oils, waxes, some dyes, other organic and inorganic compounds.	56
2,2-Dichloropropane		
2-Chlorotoluene (o-")	Used in pesticides	57
4-Chlorotoluene (p-Chloroto	Solvent, intermediate	3
4-Isopropyltoluene		

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APPENDIX A

DATA SET 2 – SVOC’s

Name	Type of chem substance	Ref	Molc weight	Ref	Solubility in water mg/L	@ T	Ref	Koc (mL/g)	Ref	Log Koc (mL/g)	Ref	Molc structure	Ref	CAS NO	Ref	Boiling Point	Ref
Acenaphthene	aromatic	8	154.21	4	3.47, 3.9		4,3	7832.493	8	3.8939	Est from Kow	$C_{12}H_{10}$	4	83-32-9	4	279	4
Acenaphthylene	aromatic	8	152.2	4	3.93, 3.9		8,3	4765.407	8	3.6781	Est from Kow	$C_{12}H_8$	4	208-96-8	4	265	4
Anthracene	aromatic	8	178.23	2	0.073, 0.0434		17, 2	11700.38	8	4.0682	Est from Kow	$C_{14}H_{10}$	4	120-12-7	8	340	4
Azobenzene			182.22	4	<100	17.5	4					$C_{12}H_{10}N_2$	4	103-33-3	4	293	4
Benzo[a]anthracene	aromatic	8	228.29	4	0.01-0.057		8	90427.39	8	4.9563	Est from Kow	$C_{18}H_{12}$	4	56-55-3	8	437.6	4
Benzo[a]pyrene	aromatic	8	252.3	2	0.003, 0.38		8	495450.2	8	5.695	Est from Kow	$C_{20}H_{12}$	4	50-32-8	8	495	4
Benzo[b]fluoranthene	aromatic	8	252	2	1.50E-03		2	1.20E+06	18			$C_{20}H_{12}$	4	205-99-2	8	357	4
Benzo[g,h,i]perylene	aromatic	8	276.34	2	2.60E-04		2	1999401	8	6.3009	Est from Kow	$C_{22}H_{12}$	4	191-24-2	8	500	4
Benzo[k]fluoranthene	aromatic	8	252	2	8e-4, 0.0043		2,8	948855.3	8	5.9772	Est from Kow	$C_{20}H_{12}$	4	207-08-9	8	480	4
bis(2-Chloroethoxy)methane	chlorinated ether	8	173.04	4	8.10E+04		8	22.17175	8	1.3458	Est from Kow	$C_5H_{10}Cl_2O_2$	4	111-91-1	4	218.1	4
bis(2-Chloroethyl)ether	chlorinated ether	8	143.01	2	1.58		8	40.86956	8	1.6114	Est from Kow	C4H8Cl2O	1	111-44-4	1	179	1
bis(2-chloroisopropyl)ether	clorinated ether	8	171.07	1	1.70E+03		1	61.6595	1	1.79	1	C6H12Cl2	1	108-60-1	1	187	1
bis(2-Ethylhexyl)phthalate	phthalate ester	8	390.56	4	0.4-1.3		8	50003.45	8	4.699	Est from Kow	$C_{24}H_{38}O_4$	4	117-81-7	8	386.9	4
Butylbenzylphthalate	phthalate ester	8	312.37	1	2.82		1	1698.244	1	3.23	1	C19H20O4	1	85-68-7	1	370	1
Carbazole	aromatic	8	167.21	4	<1000	19	4					$C_{12}H_9N$	4	86-74-8	4	355	4
Chrysene	aromatic	8	228.2	2	15		8	90427.39	8	4.9563	Est from Kow	$C_{18}H_{12}$	4	218-01-9	8	448	4
Dibenz[a,h]anthracene	hlorinated aromati	8	278.35	2	.00249, 0.0005		2,8	179928.5	8	5.2551	Est from Kow	$C_{22}H_{14}$	4	53-70-3	8	524	4
Dibenzofuran			168.19	4	<1000	20	4					$C_{12}H_8O$	4	132-64-9	4	285	4
Diethylphthalate	phthalate ester	8	222.24	1	9.28E+02		1	69.1831	1	1.84	1	C12H14O2	1	84-66-2	1	298	1
Dimethylphthalate	phthalate ester	8	194.19	4	1000, 4.29e+	20 (4)	4,1	39.33689	8	1.5948	Est from Kow	$C_{10}H_{10}O_4$	4	131-11-3	4	283.7	4
Di-n-butylphthalate	phthalate ester	8	278.35	4	13		4	41304.75	8	4.616	Est from Kow	$C_{16}H_{22}O_4$	4	84-74-2	8	340	4
Di-n-octylphthalate	phthalate ester	8	390.56	4	3		8	86297855	8	7.936	Est from Kow	$C_{24}H_{38}O_4$	4	117-84-0	8	220	4
Fluoranthene	aromatic	8	202.23	2	0.265		8	52954.15	8	4.7239	Est from Kow	$C_{16}H_{10}$	4	206-44-0	8	375	4
Fluorene	aromatic	8	166.2	2	1.98, 2		2,3	6109.42	8	3.786	Est from Kow	$C_{13}H_{10}$	4	86-73-7	8	295	4
Hexachlorobenzene	hlorinated aromati	8	284.78	4	0.0062		4					C_6Cl_6	4	118-74-1	4	332	4
Hexachlorobutadiene	chlorinated alkane	8	260.76	1	2.55		1	4677.351	1	3.67	1	C4Cl6	1	87-68-3	1	215	1
Hexachlorocyclopentadiene	pesticide	8	272.77	1	1.1		1	4265.795	1	3.63	1	C5Cl6	1	77-47-4	1	237	1
Hexachloroethane	chlorinated alkane	8	236.74	4	50, 1.8, 50		4,8,3	4089.781	8	3.6117	Est from Kow	C_2Cl_6	4	67-72-1	4	189	4
Indeno[1,2,3-cd]pyrene	chlorianted alkane	8	276.34	4	50, 0.062		8,4	1180.864	8	3.0722	Est from Kow	$C_{22}H_{12}$	4	193-39-5	8	536	4
Isophorone	aromatic	8	138.21	4	12000		4					$C_9H_{14}O$	4	78-59-1	4	215.2	4
Naphthalene	aromatic	8	128.6	2	31		2	1203.649	6	3.0805	6	C10H8	4	91-20-3	4	218	4
Nitrobenzene	substituted aromati	8	123.11	1	1900, 2500		1,8	6.50E+01	18			C6H5NO2	1	98-95-3	1	211	

Name	Type of chem substance	Ref	Molc weight	Ref	Solubility in water mg/L	@ T	Ref	Koc (mL/g)	Ref	Log Koc (mL/g)	Ref	Molc structure	Ref	CAS NO	Ref	Boiling Point	Ref
N-Nitrosodimethylamine	organic	8	74.082	4	>=100000	19	4	529.1758	8	2.7236	Est from Kow	$C_2H_6N_2O$		62-75-9		149	
N-Nitroso-di-n-propylamine	organic	8	130.19	4	9894		4	2.23769	8	0.3498	Est from Kow	$C_6H_{14}N_2O$	4	621-64-7	4	206	4
Pentachlorophenol	phenol	8	266.34	4	0.0027, 14		8,4	235125.6	8	5.3713	Est from Kow	C_6HCl_5O	4	87-86-5	8	310	4
Phenanthrene	aromatic	8	178.23	4	1.18, 1.3		5,3	11261.6	6	4.0516	6	$C_{14}H_{10}$	4	85-01-8	4	340	4
Phenol	phenol	8	94.113	4	82800		2	10041.53	8	4.0018	Est from Kow	C_6H_6O	4	108-95-2	4	181.7	4
Pyrene	aromatic	8	202.26	2	0.135, 0.013		2,4	32.49376	8	1.5118	Est from Kow	$C_{16}H_{10}$	4	129-00-0	8	404	4
1,2,4-Trichlorobenzene	chlorinated aromati	8	181.45	1	19	20	1	9549.926	1	3.98	1	C6H3C13		120-82-1		210	1
1,2-Dichlorobenzene	chlorinated aromati	8	147	1	83.96, 100	20 (1)	4,1	186.2087	1	2.27	1	C6H4Cl2	1	95-50-1	1	180	1
1,3-Dichlorobenzene	chlorinated aromati	8	147	1	1.11E+02	20 (1)	1	169.8244	1	2.23	1	C6H4Cl2	1	541-73-1	1	173	1
1,4-Dichlorobenzene	chlorinated aromati	8	147	4	81.3		4	1299.272	8	3.1137	Est from Kow	$C_6H_4Cl_2$	4	106-46-7	4	173.4	4
2,4,5-Trichlorophenol			197.45	4	1200		4					$C_6H_3Cl_3O$	4	95-95-4	4	253	4
2,4,6-Trichlorophenol	phenol	8	197.45	4	800		4	2441.181	8	3.3876	Est from Kow	$C_6H_3Cl_3O$	4	88-06-2	4	244.5	4
2,4-Dichlorophenol	phenol	8	163	4	4500		4	382.3843	8	2.5825	Est from Kow	$C_6H_4Cl_2O$	4	120-83-2	4	210	4
2,4-Dimethylphenol	phenol	8	122.17	4	7870		4	203.5167	8	2.3086	Est from Kow	$C_8H_{10}O$	4	105-67-9	4	210.9	4
2,4-Dinitrophenol	phenol	8	184.11	4	2787, 5600		4,8	35.75197	8	1.5533	Est from Kow	$C_6H_4N_2O_5$	4	51-28-5	8	113	4
2,4-Dinitrotoluene	substituted aromati	8	182.14	4	270		8	57.65009	8	1.7608	Est from Kow	$C_7H_6N_2O_4$	4	100-02-7	8	300	4
2,6-Dinitrotoluene	substituted aromati	8	182.14	4	182		4	100.346	8	2.0015	Est from Kow	$C_7H_6N_2O_4$	4	606-20-2	8	300	4
2-Chloronaphthalene	chlorinated bipheno	8	162.62	4	6.74		4	5243.243	8	3.7196	Est from Kow	$C_{10}H_7Cl$	4	91-58-7	4	256	4
2-Chlorophenol	phenol	8	128.56	4	28500		4	121.4787	8	2.0845	Est from Kow	C_6H_5ClO	4	95-57-8	8.00	175.6	4
2-Methylnaphthalene			142.2	4	24.6		4	8.50E+03	18			$C_{11}H_{10}$	4	91-57-6	4	241	4
2-Methylphenol			108.14	4	<1000	19	4					C_7H_8O	4	95-48-7	4	191	4
2-Nitroaniline			138.13	4	1260		4					$C_6H_6N_2O_2$	4	88-74-4	4	284	4
2-Nitrophenol	phenol	8	139.11	4	2100		4	68.46995	8	1.8355	Est from Kow	$C_6H_5NO_3$	4	88-75-5	4	214.6	4
3-Nitroaniline			138.13	4	890		4					$C_6H_6N_2O_2$	4	99-09-2	4	306	4
4,6-Dinitro-2-methylphenol			198.13	4	100		4					$C_7H_6N_2O_5$	4	534-52-1	4		
4-Bromophenyl-phenylether	chlorinated ether	8	249.11	4				7118.689	8	3.8524	Est from Kow	$C_{12}H_9BrO$	4	101-55-3	8	310.14	4
4-Chloro-3-methylphenol			142.58	4	3850		4					C_7H_7ClO	4	59-50-7	4	235	4
4-Chloroaniline			127.57	4	3.9		4					C_6H_6ClN	4	106-47-8	4	232	4
4-Chlorophenyl-phenylether	chlorinated ether	8	204.66	1	3.3		1	3981.072	1	3.6	1	C12H9ClO	1	7005-72-3	1	284	1
4-Methylphenol			108.14	4	<1000	21	4					C_7H_8O	4	106-44-5	4	201.8	4
4-Nitroaniline			138.13	4	800		4					$C_6H_6N_2O_2$	4	100-01-6	4	332	4
4-Nitrophenol	phenol	8	139.11	4	16000		8					C13H10					
Vinyl acetate			86	2	20000	2								108-05-4	2		

Name	Flash Point	Ref	Spec Density (gm/cm3) / (g/cc)	@ T	Ref	Absolute Viscosity	Ref	Vapor P (mm Hg)	@ T	Ref	Henry's Law Const	Ref	Log Kow (L)	Ref	Diff coeff in H2O cm2/d	Ref
Acenaphthene	125	4	1.069	N/R	4			1.00E-02	20	8	3.93-9.1e-5	8	4.33	8	6.98E-06	2
Acenaphthylene			0.899	N/R	4			1.00E-02	20	8	1.90E-04	8	4.07	8		
Anthracene	121	4	1.25	N/R	8			1.95E-04	20	8	8.60E-05	8	4.54	8		
Azobenzene	476	4	1.09	N/R	4											
Benzo[a]anthracene								5.00E-09	20	8	1.00E-06	8	5.61	8		
Benzo[a]pyrene								5.00E-09	20	8	5.00E-02	8	6.5	8		
Benzo[b]fluoranthene											1.22E-05	8				
Benzo[g,h,i]perylene								1.30E-10	20	8	1.44E-07	8	7.23	8		
Benzo[k]fluoranthene								9.59E-11	20	8	3.87E-05	8	6.84	8		
bis(2-Chloroethoxy)methane								<0.1	20	8	2.86E-07	8	1.26	8		
bis(2-Chloroethyl)ether	55		1.22			2.14	1	7.10E-01	20	1	1.30E-05	1	1.58	1		
bis(2-chloroisopropyl)ether	85	1	1.103	20	1			8.50E-01	20	1	1.10E-04	1	2.58	1		
bis(2-Ethylhexyl)phthalate	386.9	4	0.9732	N/R	4			2.00E-07	20	8	3.00E-07	8	5.3	8		
Butylbenzylphthalate	110	1	1.12	20	1			8.60E-06	20	1	1.30E-06	1	4.78	1		
Carbazole	220	4	1.1	N/R	4											
Chrysene			1.274	N/R	8			1.00E-06	20	8	1.05E-06	8	5.61	8		
Dibenz[a,h]anthracene								1.00E-10	20	8	7.30E-08	8	5.97	8		
Dibenzofuran	130	4														
Diethylphthalate	140	1	1.118	20	1	35	1	1.65E-03	20	1	8.46E-07	1	2.35	1		
Dimethylphthalate	146	4	1.19	N/R	4	9.18	8	4.20E-03	20	8	00000215, 4.2	8,1	1.56	8		
Di-n-butylphthalate	171	4	1.046	N/R	8			1.00E-05	20	8	6.3e-5, 2.8e-7	8	5.2	8		
Di-n-octylphthalate	104	4	0.978	N/R	4			1.40E-04	20	8	1.70E-05	8	9.2	8		
Fluoranthene								1.00E-04	20	8	6.50E-06	8	5.33	8		
Fluorene	151	4	1.203	N/R	8			1.00E-04	20	8	2.1e-4, 6.4e-5	8	4.2	8		
Hexachlorobenzene	242	4	2.044	N/R	4											
Hexachlorobutadiene	NC	1	1.554	20	1	2.45	1	1.50E-01	20	1	2.60E-02	1	4.78	1		
Hexachlorocyclopentadiene	NC	1	1.702	20	1			8.10E-02	20	1	1.60E-02	1	5.04	1		
Hexachloroethane			1.702, 2.09	N/R	8,3			0.081	20	8	1.60E-02	8	3.99	8		
Indeno[1,2,3-cd]pyrene			2.09	N/R	8			4.00E-01	20	8			3.34	8		
Isophorone	84	4	0.9229	N/R	4											
Naphthalene	78	4	0.997	N/R	4			4.42		4	36.6-74.4	12	3.35	6		
Nitrobenzene	88		1.024	20	1	2.01		1.50E-01	20	1	2.45E-05	1				

Name	Flash Point	Ref	Spec Density (gm/cm3) / (g/cc)	@ T	Ref	Absolute Viscosity	Ref	Vapor P (mm Hg)	@ T	Ref	Henry's Law Const	Ref	Log Kow (L)	Ref	Diff coeff in H2O cm2/d	Ref
N-Nitrosodimethylamine	61		1.006					2.2	20	8	2.50E-05	8	2.92	8		
N-Nitroso-di-n-propylamine	99	4						8.1	20	8	2.30E-05	8	0.06	8		
Pentachlorophenol			1.979	N/R	4			4.05E-05	20	8	6.1-7.1e-5	8	6.11	8		
Phenanthrene			1.063	N/R	4						0.0016 - 0.0003	5	4.52	6		
Phenol	79	4	1.07	N/R	4			0.35		4	1.3-2.3e-4	8	4.46	8		
Pyrene	210	4	1.07	N/R	8			0.2-0.53	20	8	2.7-4.5E-7	8	1.46	8		
1,2,4-Trichlorobenzene	105	1	1.4	20	1	1.42	1	4.00E-01	20	1	2.32E-03	1	4.02	1		
1,2-Dichlorobenzene	67	4	1.305	20	1	1.32	1	1	20	1	1.90E-03	1	3.4	1		
1,3-Dichlorobenzene	63	1	1.288	20	1	1.04	1	2.3	20	1	3.60E-03	1	3.38	1		
1,4-Dichlorobenzene	67	4	1.2417	N/R	4	0.72	8	0.4		4	2.1-3e-3	8	3.39	8		
2,4,5-Trichlorophenol			1.5	N/R	4											
2,4,6-Trichlorophenol	99	4	1.49	N/R	4			0.012	20	8	4.00E-06	8	3.72	8		
2,4-Dichlorophenol	113	4	1.383	N/R	4			0.12	20	8	4.2e-5, 2.8e-6	8	2.75	8		
2,4-Dimethylphenol	110	4	0.965	N/R	4			0.0621	20	8	1.70E-05	8	2.42	8		
2,4-Dinitrophenol			1.683	N/R	8			1.49E-05	20	8	6.45E-10	8	1.51	8		
2,4-Dinitrotoluene	206.7	4	1.675	N/R	8			1	20	8	7.60E-05	8	1.76	8		
2,6-Dinitrotoluene			1.2833	N/R	4			0.018	20	8	1.00E-06	8	2.05	8		
2-Chloronaphthalene			1.2656	N/R	4			0.017	20	8	5.40E-04	8	4.12	8		
2-Chlorophenol	63	4	1.241	N/R	8	2.25	8	2.2	20	8	2.1e-5, 8.28e-	8,1	2.15	8		
2-Methylnaphthalene	97	4	1	N/R	4											
2-Methylphenol	81	4	1.048	N/R	4											
2-Nitroaniline	168	4	1.422	N/R	4											
2-Nitrophenol	102	4	1.495	N/R	4	1.634	8	0.15	20	8	1.10E-05	8	1.85	8		
3-Nitroaniline			1.43	N/R	4											
4,6-Dinitro-2-methylphenol																
4-Bromophenyl-phenylether			1.423	N/R	8			1.50E-03	20	8	1.00E-04	8	4.28	8		
4-Chloro-3-methylphenol	118	4														
4-Chloroaniline			1.17	N/R	4											
4-Chlorophenyl-phenylether			1.203	20	1			2.70E-03	20	1	2.20E-04	1	4.08	1		
4-Methylphenol	89	4	1.034	N/R	4			0.1		4						
4-Nitroaniline	199	4														
4-Nitrophenol																
Vinyl acetate											0	2	1	2	0	2

Name	Heat of Vapor kJ/mol 25 degr celc	Surface tension dyn/cm	Ref	Interfacial tension dyn/cm	Kd determinable	Half life soil (days)	Ref	Half life GW (days)	Ref
Acenaphthene					1				
Acenaphthylene					1				
Anthracene					1				
Azobenzene					0				
Benzo[a]anthracene					1				
Benzo[a]pyrene					1				
Benzo[b]fluoranthene					1				
Benzo[g,h,i]perylene					1	3.2-3.6 y	8		
Benzo[k]fluoranthene					1				
bis(2-Chloroethoxy)methane					1				
bis(2-Chloroethyl)ether		37.9	1		1	28-180	1	56-360	1
bis(2-chloroisopropyl)ether					1	18-180	1	36-360	1
bis(2-Ethylhexyl)phthalate					1				
Butylbenzylphthalate					1	1.-7	1	2-180	1
Carbazole					0				
Chrysene					1				
Dibenz[a,h]anthracene					1				
Dibenzofuran					0				
Diethylphthalate		37.5	1		1	3.-56	1	6-112	1
Dimethylphthalate					1	1.-7	1	2.-14	1
Di-n-butylphthalate					1				
Di-n-octylphthalate					1				
Fluoranthene					1				
Fluorene					1				
Hexachlorobenzene					0				
Hexachlorobutadiene					1	28-181	1	56-361	1
Hexachlorocyclopentadiene		37.5	1		1	7.-28	1	7.-56	1
Hexachloroethane					1				
Indeno[1,2,3-cd]pyrene					1				
Isophorone					0				
Naphthalene					1				
Nitrobenzene		43	1	25.7	1	12-197	1	2-394	1

Name	Heat of Vapor kJ/mol 25 degr celc	Surface tension dyn/cm	Ref	Interfacial tension dyn/cm	Kd determinable	Half life soil (days)	Ref	Half life GW (days)	Ref
N-Nitrosodimethylamine					1				
N-Nitroso-di-n-propylamine					1				
Pentachlorophenol					1	21-1087	8		
Phenanthrene	72.5				1				
Phenol					1				
Pyrene					1				
1,2,4-Trichlorobenzene		39.1	1		1	28-180	1	56-360	1
1,2-Dichlorobenzene	61.51	37	1	40	1	28-180	1	56-360	1
1,3-Dichlorobenzene		33.2	1		1	28-180	1	56-360	1
1,4-Dichlorobenzene					1				
2,4,5-Trichlorophenol					0				
2,4,6-Trichlorophenol					1				
2,4-Dichlorophenol					1				
2,4-Dimethylphenol					1				
2,4-Dinitrophenol					1				
2,4-Dinitrotoluene					1				
2,6-Dinitrotoluene					1				
2-Chloronaphthalene					1				
2-Chlorophenol		40.3	1		1				
2-Methylnaphthalene					1				
2-Methylphenol					0				
2-Nitroaniline					0				
2-Nitrophenol					1				
3-Nitroaniline					0				
4,6-Dinitro-2-methylphenol					0				
4-Bromophenyl-phenylether					1				
4-Chloro-3-methylphenol					0				
4-Chloroaniline					0				
4-Chlorophenyl-phenylether					1				
4-Methylphenol					0				
4-Nitroaniline					0				
4-Nitrophenol					0	14-28	8		
Vinyl acetate					0				

Name	Usage	Ref
Acenaphthene	Coal tar by-product	3
Acenaphthylene	Coal tar by-product	3
Anthracene	Dyestuffs, intermediate, semiconductor research, coal tar by-product	3
Azobenzene	Intermediate for azo dyes and other organic chemicals, acaracide	19
Benzo[a]anthracene	coal-tar by-product	3
Benzo[a]pyrene	coal tar by-product	3
Benzo[b]fluoranthene	coal tar by-product	3
Benzo[g,h,i]perylene	coal tar by-product	3
Benzo[k]fluoranthene	coal tar by-product	3
bis(2-Chloroethoxy)methane	High volume chemical; used as a starting compound to produce polysulfide elastomers. Also used as solvent.	20; 21
bis(2-Chloroethyl)ether	Chemical intermediate for pesticides manufacture.Small amount used as a solvent. Past uses: solvent for fats, waxes, greases, and esters, constituent of paints & varnishes, cleaning fluid for textiles, purification of oils and gasoline.	22
bis(2-chloroisopropyl)ether	Past use: Intermediate of dyes, resins & pharmaceuticals, textile processes; current use: nematocide (Japan). Combatant in liver fluke infections, preparation of glycol esters, fungicidal preparations, insecticidal wood preservative. Solvent (fats, paint)	23
bis(2-Ethylhexyl)phthalate	Production: PVC & vinyl chloride resins, where it is added to plastics to make them flexible.	24
Butylbenzylphthalate	printing inks; plasticisers in many plastics, in products such as baby milk formula, cheese, margarine and crisps	25; 26
Carbazole	Dye intermediate, mfr. Of explosive tetranitrocarbazoel, photographic plates.	27
Chrysene	organic synthesis, coal-tar by-product	3
Dibenz[a,h]anthracene	NA	
Dibenzofuran	Naturally occuring in coal tar, component of heat transfer oils, polymer production & dyeing, printing of textiles, air releases due to incomplete combustion of coal & oil products.	28
Diethylphthalate	Manufacture of celluloid, cosmetics, varnishes, dopes, plasticiser for cellulose ester plastics, insecticide sprays.	29
Dimethylphthalate	Used in solid rocket propellants, lacquers, plastics, safety glasses, rubber coating agents, molding powders, insect repellants, and pesticides.	30
Di-n-butylphthalate	insect repellent for clothing; plasticizer for elastomers, lacquers, solid rocket propellents, and nail polishes; perfume solvent, safety glass, adhesives.	31
Di-n-octylphthalate	Plasticizer for polyvinyl chloride and other vinyls	3
Fluoranthene	Intermediate for dyes(fluorescent), pharmaceuticals and agrochemicals.	32
Fluorene	Resinous products, dyestuffs, insecticides, coal tar by-product	3
Hexachlorobenzene	Past use: pesticide to protect the seeds of onions and sorghum, wheat, and other grains against fungus until 1965. IAlso used to make fireworks, ammunition, and synthetic rubber.	33
Hexachlorobutadiene	Solvent, transformer and hydraulic fluid, heat transfer liquid	3
Hexachlorocyclopentadiene	Intermediate for resins, dyestuffs, pesticides, fungicides, pharmaceuticals	3
Hexachloroethane	Solvent, pyrotechnics and smoke devices, explosives, organic synthesis	3
Indeno[1,2,3-cd]pyrene		
Isophorone	Solvent for vinyl chloride/acetate-based coating, nitrocellulose finishes,printing inks for plastics, used in herbicide & pesticide formulations & adhesives, intermediate	34
Naphthalene	Solvent, lubricant, expolsives, preservatives, intermediate, fungicide, moth repellant, coal tar by product, gasoline	3
Nitrobenzene	Solvent, polishes, chemical manufacturing	3

Name	Usage	Ref
N-Nitrosodimethylamine	Pesticides, retarder of vulcunization of rubber	3
N-Nitroso-di-n-propylamine	Production of rubber products	35
Pentachlorophenol	Used as insecticide (termiticide), fungicide, herbicide, molluscicide, algicide, disinfectant, wood preservative.	36
Phenanthrene	Dyestuffs, expolsives, synthesis of drugs, biochemical research	3
Phenol		3
Pyrene	Biochemical research, coal tar by-product	3
1,2,4-Trichlorobenzene	Dye carrier, herbicide intermediate, heat-transfer medium, dielectric fluid in transformers, degreaser, lubricant, in synthetic transformer oils, as solvent in chemical manufacturing, Formerly used as insecticide against termites.	37
1,2-Dichlorobenzene	Chemical intermediate and as a solvent, production of chemicals and herbicide, metal, leather and wool degreaser.	38
1,3-Dichlorobenzene	It is used as a fumigant and insecticide	39
1,4-Dichlorobenzene		40
2,4,5-Trichlorophenol	Algecide, microbiocide	41
2,4,6-Trichlorophenol	Herbicide, past use preservative & disinfectant, bactericide, fungicide, sanitizer, wood & glue preservative, insecticide ingredient.	42
2,4-Dichlorophenol	Organic synthesis	3
2,4-Dimethylphenol	Pharmaceuticals, plastics, disinfectants, solvent, dyestuffs, insecticides, fungicides, additives to lubricants & gasolines	3
2,4-Dinitrophenol	Herbicides	3
2,4-Dinitrotoluene	Intermediate for toluene, gelatanizing & waterproofing agent in explosives, intermediate for dyes, rubber chemical and plastics manufacture. Used as a plasticizer in moderate and high explosives.	43
2,6-Dinitrotoluene	Intermediate for toluene, gelatinizing & waterproofing agent in explosives, synthesis of TNT, urethane polymers, flexible and rigid foams, surface coatings and dyes	44
2-Chloronaphthalene	Plasticizer, solvent for dyestuffs, varnish gums and resins, waxes, moisture-, flame-, acid-, and insect-proofing of fibrous materials, moisture- and flame-prrofing of electrical cable	3
2-Chlorophenol	Org synthesis (dyes), disinfectant formulations, intermediate in manufacture of dyestuffs & preservatives, disinfectant/bacteriocide/germicide	45
2-Methylnaphthalene	Organic synthesis, insecticides, dye carrier,used for vitamin K production and as a chemical intermediate	46
2-Methylphenol	Solvent or disinfectant, chemical intermediate, maufacture of dye intermediates,	47
2-Nitroaniline	Intermediate for pigment yellow, orange, vat red, synthesis of photographic antifogging agent	48
2-Nitrophenol		49
3-Nitroaniline		
4,6-Dinitro-2-methylphenol		
4-Bromophenyl-phenylether		
4-Chloro-3-methylphenol		
4-Chloroaniline		
4-Chlorophenyl-phenylether		
4-Methylphenol		
4-Nitroaniline		
4-Nitrophenol	Chemical manufacturing	3
Vinyl acetate		

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1,2-Dibromoethane: Ashworth et al (1988) in Pa m3 / g mol
n-propylbenzene: ashworth et al (1988) in Pa m3 / g mol
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29 National Toxicology Program: http://ntp-server.niehs.nih.gov/htdocs/Levels/Tr429levels.Html
30 EPA: http://www.epa.gov/ttn/atw/hlthef/dimet-ph.html
31 Biospace: http://biospace.intota.com/multisearch.asp?mode=&strSearchType=all&strQuery=di-n-butylphthalate
32 ChemicalLand21: http://www.chemicalland21.com/arokorhi/specialtychem/finechem/FLUORANTHENE.htm
33 ATSDR: http://www.atsdr.cdc.gov/tfacts90.html
34 EPA: http://www.epa.gov/ttn/atw/hlthef/isophoro.html
35 US Dept of Labour: http://www.osha.gov/dts/hib/hib_data/hib19891010.html
36 ATSDR: http://www.atsdr.cdc.gov/toxprofiles/tp51-c5.pdf
37 EPA: http://www.epa.gov/ttnatw01/hlthef/tri-zene.htm
38 EPA: http://www.oehha.ca.gov/water/phg/pdf/12dcb_c.pdf
39 Cheminfo: http://gis.wvdep.org/tri/cheminfo/csfs149.txt
40 ATSDR: http://www.atsdr.cdc.gov/tfacts10.html
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47 ATSDR: http://64.233.167.104/search?q=cache:KmWnhlcFDFIJ:www.atsdr.cdc.gov/toxprofiles/
tp34-c4.pdf+cresol+use&hl=en&ie=UTF-8
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APPENDIX B

MOST STRINGENT ORGANIC WATER QUALITY STANDARDS

Most Stringent Water Quality Guidelines - SVOC

CHEMICAL CONSTITUENT	Most Stringent Water Quality Guideline				EPA Drinking Water Standards			Dutch Intervention values		Massachusetts Drinking Water Standards	WHO Drinking Water Standard
	COMPLIANCE CLASSIFICATION			WATER QUALITY CRITERIUM USED FOR COMPLIANCE	COMPLIANCE CLASSIFICATION		CANCER GROUP	COMPLIANCE CLASSIFICATION		COMPLIANCE CLASSIFICATION	COMPLIANCE CLASSIFICATION
	FULL COMPLIANCE (mg/l)	MARGINAL COMPLIANCE (mg/l)	NON-COMPLIANCE (mg/l)		MCLG (mg/l)	MCL (mg/l)		TARGET VALUE (mg/l)	INTERVENTION VALUE (mg/l)	MMCL (mg/l)	GUIDELINE VALUE (mg/l)
1,2,4-Trichlorobenzene	<0.00001	0.00001 - 0.01	>0.01	Dutch Intervention Standard	0.07	0.07	D	0.00001	0.01	0.07	0.02
1,2-Dichlorobenzene	<0.00001	0.00001 - 0.05	>0.05	Dutch Intervention Standard	N.S.	N.S.		0.00001	0.05	0.6	1
1,3-Dichlorobenzene	<0.00001	0.00001 - 0.05	>0.05	Dutch Intervention Standard	N.S.	N.S.		0.00001	0.05	N.S.	N.S.
1,4-Dichlorobenzene	<0.00001	0.00001 - 0.05	>0.05	Dutch Intervention Standard	N.S.	N.S.		0.00001	0.05	0.005	0.3
2,4,5-Trichlorophenol	<0.000025	0.000025 - 0.01	>0.01	Dutch Intervention Standard	N.S.	N.S.		0.000025	0.01	N.S.	N.S.
2,4,6-Trichlorophenol	<0.000025	0.000025 - 0.01	>0.01	Dutch Intervention Standard	N.S.	N.S.	B2	0.000025	0.01	N.S.	0.002
2,4-Dichlorophenol	<0.00008	0.00008 - 0.03	>0.03	Dutch Intervention Standard	N.S.	N.S.	B3	0.00008	0.03	N.S.	0.0003
2,4-Dimethylphenol	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
2,4-Dinitrophenol	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
2,4-Dinitrotoluene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	B2	N.S.	N.S.	N.S.	N.S.
2,6-Dinitrotoluene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	B2	N.S.	N.S.	N.S.	N.S.
2-Chloronaphthalene	<0.006	N.S.	>0.006	No Standard Available	N.S.	N.S.		N.S.	0.006	N.S.	N.S.
2-Chlorophenol	<0.0001	N.S.	>0.0001	WHO Drinking Water Standard	N.S.	N.S.		0.00025	0.1	N.S.	0.0001
2-Methylnaphthalene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
2-Methylphenol	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
2-Nitroaniline	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
2-Nitrophenol	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
3-Nitroaniline	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
4,6-Dinitro-2-methylphenol	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
4-Bromophenyl-phenylether	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
4-Chloro-3-methylphenol	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
4-Chloroaniline	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
4-Chlorophenyl-phenylether	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
4-Methylphenol	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
4-Nitroaniline	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
4-Nitrophenol	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
Acenaphthene	N.S.	N.S.	N.S.	Dutch Intervention Standard	N.S.	N.S.	-	N.S.	N.S.	N.S.	N.S.
Acenaphthylene	N.S.	N.S.	N.S.	Dutch Intervention Standard	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
Anthracene	<0.00002	0.00002 - 0.005	>0.005	Dutch Intervention Standard	N.S.	N.S.	D	0.00002	0.005	N.S.	N.S.
Azobenzene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
Benzo[a]anthracene	<0.000002	0.000002 - 0.0005	>0.0005	Dutch Intervention Standard	N.S.	N.S.	B2	0.000002	0.0005	N.S.	N.S.
Benzo[a]pyrene	<0.000001	0.000001 - 0.00005	>0.00005	Dutch Intervention Standard	0	0.0002	B2	0.000001	0.00005	0.0002	0.0007

MCLG - Maximum Contaminant Level Goal
MCL - Maximum Contaminant Level
A - Human Carcinogen
B2 - Probable human carcinogen - sufficient evidence in animals & inadequete or no evidence in humans
C - Possible human carcinogen
D - Not Classifiable as to human carcinogenity

Most Stringent Water Quality Guideline Values were compiled using most stringent guideline for each variable
Poly Aromatic Hydrocarbons
SA Water Quality Guideline - Domestic use - phenol target value = 1mg/l

Most Stringent Water Quality Guidelines - SVOC contd.

	Most Stringent Water Quality Guideline				EPA Drinking Water Standards			Dutch Intervention values		Massachusetts Drinking Water Standards	WHO Drinking Water Standard
	COMPLIANCE CLASSIFICATION			WATER QUALITY CRITERIUM USED FOR COMPLIANCE	COMPLIANCE CLASSIFICATION		CANCER GROUP	COMPLIANCE CLASSIFICATION		COMPLIANCE CLASSIFICATION	COMPLIANCE CLASSIFICATION
CHEMICAL CONSTITUENT	FULL COMPLIANCE (mg/l)	MARGINAL COMPLIANCE (mg/l)	NON-COMPLIANCE (mg/l)		MCLG (mg/l)	MCL (mg/l)		TARGET VALUE (mg/l)	INTERVENTION VALUE (mg/l)	MMCL (mg/l)	GUIDELINE VALUE (mg/l)
Benzo[b]+[K]fluoranthene	N.S.	N.S.	N.S.	Dutch Intervention Standard	N.S.	N.S.	B2	N.S.	N.S.	N.S.	N.S.
Benzo[g,h,i]perylene	<0.0000002	0.0000002 - 0.00005	>0.00005	Dutch Intervention Standard	N.S.	N.S.	D	0.0000002	0.00005	N.S.	N.S.
bis(2-Chloroethoxy)methane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
bis(2-Chloroethyl)ether	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
bis(2-chloroisopropyl)ether	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
bis(2-Ethylhexyl)phthalate	<0.0005	0.0005 - 0.005	>0.005	Dutch Intervention Standard	N.S.	N.S.		0.0005	0.005	0.006	0.008
Butylbenzylphthalate	<0.0005	0.0005 - 0.005	>0.005	Dutch Intervention Standard	N.S.	N.S.	C	0.0005	0.005	N.S.	N.S.
Carbazole	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
Chrysene	<0.000002	0.000002 - 0.00005	>0.00005	Dutch Intervention Standard	N.S.	N.S.	B2	0.000002	0.00005	N.S.	N.S.
Dibenz[a,h]anthracene	N.S.	N.S.	N.S.	Dutch Intervention Standard	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
Dibenzofuran	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
Diethylphthalate	<0.0005	0.0005 - 0.005	>0.005	Dutch Intervention Standard	N.S.	N.S.	D	0.0005	0.005	N.S.	N.S.
Dimethylphthalate	<0.0005	0.0005 - 0.005	>0.005	Dutch Intervention Standard	N.S.	N.S.	D	0.0005	0.005	N.S.	N.S.
Di-n-butylphthalate	<0.0005	0.0005 - 0.005	>0.005	Dutch Intervention Standard	N.S.	N.S.		0.0005	0.005	N.S.	N.S.
Di-n-octylphthalate	<0.0005	0.0005 - 0.005	>0.005	Dutch Intervention Standard	N.S.	N.S.		0.0005	0.005	N.S.	N.S.
Fluoranthene	<0.000005	0.000005 - 0.001	>0.001	Dutch Intervention Standard	N.S.	N.S.		0.000005	0.001	N.S.	N.S.
Fluorene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
Hexachlorobenzene	<0.00001	0.00001 - 0.0005	>0.0005	Dutch Intervention Standard	0	0.001	B2	0.00001	0.0005	0.001	N.S.
Hexachlorobutadiene	<0.0006	N.S.	>0.0006	WHO Drinking Water Standard	N.S.	N.S.	C	N.S.	N.S.	N.S.	0.0006
Hexachlorocyclopentadiene	<0.05	N.S.	>0.05	EPA Drinking Water Standard	0.05	0.05	D	N.S.	N.S.	0.05	N.S.
Hexachloroethane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	C	N.S.	N.S.	N.S.	N.S.
Indeno[1,2,3-cd]pyrene	<0.0000004	0.0000004 - 0.00005	>0.00005	Dutch Intervention Standard	N.S.	N.S.	B2	0.0000004	0.00005	N.S.	N.S.
Isophorone	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	C	N.S.	N.S.	N.S.	N.S.
Naphthalene	<0.0001	0.0001 - 0.07	>0.07	Dutch Intervention Standard	N.S.	N.S.	C	0.0001	0.07	0.14	N.S.
Nitrobenzene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
N-Nitrosodimethylamine	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
N-Nitroso-di-n-propylamine	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
Pentachlorophenol	0	0 - 0.001	>0.001	EPA Drinking Water Standard	0	0.001	B2	N.S.	N.S.	0.001	N.S.
Phenanthrene	<0.00002	0.00002 - 0.005	>0.005	Dutch Intervention Standard	N.S.	N.S.	D	0.00002	0.005	N.S.	N.S.
Phenol	<0.0002	0.0002 - 2	>2	Dutch Intervention Standard	N.S.	N.S.	D	0.0002	2	N.S.	N.S.
Pyrene	N.S.	N.S.	N.S.	Dutch Intervention Standard	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.

MCLG - Maximum Contaminant Level Goal
MCL - Maximum Contaminant Level
A - Human Carcinogen
B2 - Probable human carcinogen - sufficient evidence in animals & inadequete or no evidence in humans
C - Possible human carcinogen
D - Not Classifiable as to human carcinogenity

Most Stringent Water Quality Guideline Values were compiled using most stringent guideline for each variable
Poly Aromatic Hydrocarbons
SA Water Quality Guideline - Domestic use - phenol target value = 1mg/l

Most Stringent Water Quality Guidelines - VOC

	Most Stringent Water Quality Guideline				EPA Drinking Water Standards			Dutch Intervention values		Massachusetts Drinking Water Standards	WHO Drinking Water Standard
	COMPLIANCE CLASSIFICATION				COMPLIANCE CLASSIFICATION			COMPLIANCE CLASSIFICATION		COMPLIANCE CLASSIFICATION	COMPLIANCE CLASSIFICATION
CHEMICAL CONSTITUENT	FULL COMPLIANCE (mg/l)	MARGINAL COMPLIANCE (mg/l)	NON-COMPLIANCE (mg/l)	WATER QUALITY CRITERIUM USED FOR COMPLIANCE	MCLG (mg/l)	MCL (mg/l)	CANCER GROUP	TARGET VALUE (mg/l)	INTERVENTION VALUE (mg/l)	MMCL (mg/l)	GUIDELINE VALUE (mg/l)
1,1,1,2-Tetrachloroethane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	C	N.S.	N.S.	N.S.	N.S.
1,1,1-Trichloroethane	<0.2	N.S.	>0.2	EPA Drinking Water Standard	0.2	0.2	D	N.S.	N.S.	0.2	2
1,1,2,2-Tetrachloroethane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	C	N.S.	N.S.	N.S.	N.S.
1,1,2-Trichloroethane	<0.003	N.S.	>0.005	EPA Drinking Water Standard	0.003	0.005	C	N.S.	N.S.	0.005	N.S.
1,1-Dichloroethane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
1,1-Dichloroethene	<0	0 - 0.005	>0.005	EPA Drinking Water Standard	0	0.005	B2	N.S.	N.S.	N.S.	0.03
1,1-Dichloropropene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
1,2,3-Trichlorobenzene	<0.00001	0.00001 - 0.01	>0.01	Dutch Intervention Standard	N.S.	N.S.		0.00001	0.01	N.S.	N.S.
1,2,3-Trichloropropane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	-	N.S.	N.S.	N.S.	N.S.
1,2,4-Trichlorobenzene	<0.00001	0.00001 - 0.01	>0.01	Dutch Intervention Standard	0.07	0.07	D	0.00001	0.01	0.07	N.S.
1,2,4-Trimethylbenzene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
1,2-Dibromo-3-chloropropane	<0.0001	N.S.	>0.0001	WHO Drinking Water Standard	N.S.	N.S.		N.S.	N.S.	0.0002	0.0001
1,2-Dibromoethane	<0.0004	N.S.	>0.0004	WHO Drinking Water Standard	N.S.	N.S.		N.S.	N.S.	N.S.	0.0004
1,2-Dichlorobenzene	<0.00001	0.00001 - 0.4	>0.4	Dutch Intervention Standard	N.S.	N.S.		0.00001	0.05	0.6	1
1,2-Dichloroethane	<0	0 - 0.005	>0.005	EPA Drinking Water Standard	0	0.005	B2	0.00001	0.4	0.005	0.03
1,2-Dichloropropane	<0	1 - 0.005	>0.005	EPA Drinking Water Standard	0	0.005	B2	N.S.	N.S.	0.005	0.04
1,3,5-Trimethylbenzene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
1,3-Dichlorobenzene	<0.00001	0.00001 - 0.05	0.05	Dutch Intervention Standard	N.S.	N.S.		0.00001	0.05	N.S.	N.S.
1,3-Dichloropropane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
1,4-Dichlorobenzene	<0.00001	0.00001 - 0.05	0.05	Dutch Intervention Standard	N.S.	N.S.		0.00001	0.05	0.005	0.3
2,2-Dichloropropane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
2-Chlorotoluene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
4-Chlorotoluene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
4-Isopropyltoluene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
Benzene	<0.0002	0.0002 - 0.003	>0.003	Dutch Intervention Standard	0	0.005	A	0.0002	0.003	N.S.	0.01

MCLG - Maximum Contaminant Level Goal
MCL - Maximum Contaminant Level
A - Human Carcinogen
B2 - Probable human carcinogen - sufficient evidence in animals & inadequete or no evidence in humans
C - Possible human carcinogen
D - Not Classifiable as to human carcinogenity

Most Stringent Water Quality Guideline Values were compiled using most stringent guideline for each variable

BTEX

Most Stringent Water Quality Guidelines - VOC (contd.)

	Most Stringent Water Quality Guideline				EPA Drinking Water Standards			Dutch Intervention values		Massachusetts Drinking Water Standards	WHO Drinking Water Standard
	COMPLIANCE CLASSIFICATION			WATER QUALITY CRITERION USED FOR COMPLIANCE	COMPLIANCE CLASSIFICATION		CANCER GROUP	COMPLIANCE CLASSIFICATION		COMPLIANCE CLASSIFICATION	COMPLIANCE CLASSIFICATION
CHEMICAL CONSTITUENT	FULL COMPLIANCE (mg/l)	MARGINAL COMPLIANCE (mg/l)	NON-COMPLIANCE (mg/l)		MCLG (mg/l)	MCL (mg/l)		TARGET VALUE (mg/l)	INTERVENTION VALUE (mg/l)	MMCL (mg/l)	GUIDELINE VALUE (mg/l)
Bis(2-chloroethyl)ether	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	-	N.S.	N.S.	N.S.	N.S.
Bromobenzene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
Bromochloromethane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
Bromodichloromethane	<0	0 - 0.08	>0.08	EPA Drinking Water Standard	0	0.08	B2	N.S.	N.S.	N.S.	N.S.
Bromoform	<0	0 - 0.08	>0.08	EPA Drinking Water Standard	0	0.08	B2	N.S.	N.S.	N.S.	0.1
Bromomethane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
Carbon tetrachloride	<0	0 - 0.005	>0.005	EPA Drinking Water Standard	0	0.005	B2	N.S.	N.S.	0.005	0.002
Chlorobenzene	<0.1	N.S.	>0.1	EPA Drinking Water Standard	0.1	0.1	-	N.S.	N.S.	0.1	N.S.
Chlorodibromomethane	<0.06	N.S.	>0.06	WHO Drinking Water Standard	N.S.	N.S.	-	N.S.	N.S.	N.S.	0.06
Chloroform	<0	0 - 0.08	>0.08	EPA Drinking Water Standard	0	0.08	B2	N.S.	N.S.	N.S.	0.2
cis-1,2-Dichloroethene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
Dibromochloromethane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
Dibromomethane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
Dichlorodifluoromethane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
Dichloromethane	<0	0 - 0.005	> 0.005	EPA Drinking Water Standard	0	0.005	B2	0.00001	1	0.005	0.02
Ethylbenzene	<0.0002	0.0002 - 0.015	>0.015	Dutch Intervention Standard	0.7	0.7	D	0.0002	0.015	0.7	0.3
Hexachlorobutadiene	<0.0006	N.S.	0.0006	WHO Drinking Water Standard	N.S.	N.S.	C	N.S.	N.S.	N.S.	0.0006
Isopropylbenzene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
m,p-Xylene	<0.0002	0.0002 - 0.07	>0.07	Dutch Intervention Standard	10	10	D	0.0002	0.07	N.S.	0.5
Naphthalene	<0.0001	0.0001 - 0.07	>0.07	Dutch Intervention Standard	N.S.	N.S.	C	0.0001	0.07	0.14	N.S.
n-Butylbenzene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
n-propylbenzene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
o-dichlorobenzene	<0.00001	0.00001 - 0.05	>0.05	Dutch Intervention Standard	0.6	0.6	D	0.00001	0.05	N.S.	N.S.
o-Xylene	<0.0002	0.0002 - 0.07	>0.07	Dutch Intervention Standard	10	10	D	0.0002	0.07	N.S.	0.5
p/m-dichlorobenzene	<0.00001	0.00001 - 0.05	>0.05	Dutch Intervention Standard	0.075	0.075	C	0.00001	0.05	N.S.	N.S.
sec-Butylbenzene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
Styrene	<0.0005	0.0005 - 0.005	0.005	Dutch Intervention Standard	0.1	0.1	C	0.0005	0.005	N.S.	0.02
tert-Butylbenzene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
Tetrachloroethene	<0.00001	0.00001 - 0.04	0.04	Dutch Intervention Standard	N.S.	N.S.		0.00001	0.04	N.S.	0.04
Tetrachloroethylene	<0	0 - 0.005	>0.005	EPA Drinking Water Standard	0	0.005	-	N.S.	N.S.	0.005	N.S.
Toluene	<0.0002	0.0002 - 0.1	>0.1	Dutch Intervention Standard	1	1	D	0.0002	0.1	N.S.	0.7
trans-1,2-Dichloroethene	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.		N.S.	N.S.	N.S.	N.S.
trans-1,2-dichloroethylene	<0.1	N.S.	>0.1	EPA Drinking Water Standard	0.1	0.1	-	N.S.	N.S.	N.S.	N.S.
Trichloroethene	<0.00001	0.00001 - 0.5	0.5	Dutch Intervention Standard	N.S.	N.S.		0.00001	0.5	N.S.	0.07
Trichloroethylene / Bromodichloromethane	<0	0 - 0.08	>0.08	EPA Drinking Water Standard	0	0.08	B2	N.S.	N.S.	0.005	N.S.
Trichlorofluoromethane	N.S.	N.S.	N.S.	No Standard Available	N.S.	N.S.	D	N.S.	N.S.	N.S.	N.S.
Vinyl chloride	<0	0 - 0.002	0.002	EPA Drinking Water Standard	0	0.002	A	N.S.	0.0007	0.002	0.005

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MCL - Maximum Contaminant Level
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BTEX

APPENDIX C

ORGANIC CONTAMINANT TYPE IDENTIFICATION

Organic contaminant type identification

	Benzene ppb	M-xylene ppb	Ethylbenzene ppb	Napthalene ppb
B1	DL	DL	DL	50
B2	DL	DL	DL	40
B3	DL	DL	DL	50
B4	DL	DL	DL	40
B5	9	76	15	13000
B6	17	88	15	10200
B7	DL	DL	DL	175
B8	DL	2	2	65
B9	120	180	50	20900
B10	DL	DL	DL	DL
B11	DL	DL	DL	DL
R 1	DL	41	7	10
R 2	DL	DL	DL	8
S1	200	1130	234	47000
S2	116	570	242	25000
Totals	462	2087	565	116538
Total Xylene and Ethylbenzene (ppb)			2652	
Total all (ppb)				119652
Normalized values	0.003861197		0.022164276	0.973974526

Benzene normalized	M-xylene normalized	Ethylbenzene normalized	Napthalene normalized	Total all variables (ppb)
			1	50
			1	40
			1	50
			1	40
0.000687023	0.005801527	0.001145038	0.992366412	13100
0.001647287	0.008527132	0.001453488	0.988372093	10320
			1	175
	0.028985507	0.028985507	0.942028986	69
0.005647059	0.008470588	0.002352941	0.983529412	21250
				0
				0
	0.706896552	0.120689655	0.172413793	58
			1	8
0.004118277	0.023268265	0.004818384	0.967795075	48564
0.004473928	0.021983956	0.009333539	0.964208578	25928
0.003861197	0.017442249	0.004722027	0.973974526	119652

APPENDIX D

FRACTURE APERTURE, ENTRY PRESSURE AND NAPL POOL HEIGHT CALCULATIONS

BH ID	factor1	factor2	factor3	factor4	k1 [m/s]	k2 [m/s]	k3 [m/s]	k4 [m/s]	FlowZone	FlowZone	FlowZone	FlowZone	Aperture 1	Aperture2	Aperture3	Aperture4
BH1	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0
BH2	0.3333	0.3333	0.3333	0	0	0	0	0	2	2	1.8	0	0	0	0	0
BH3	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
BH4	0.5	0.5	0	0	0	0	0	0	0.5	0.6	0	0	0	0	0	0
BH5	0.142857	0.857143	0	0	0	0	0	0	1	1	0	0	0	0	0	0
BH6	0.041096	0.136986	0.273973	0.547945	0	0	0	0	1	1	0.5	3	0	0	0	0
BH7	0.5	0.5	0	0	0	0	0	0	1	1	0	0	0	0	0	0
BH8	0.333333	0.666667	0	0	0	0	0	0	1	2	0	0	0	0	0	0
BH9	0.038462	0.961538	0	0	0	0	0	0	1	3	0	0	0	0	0	0
BH10	0.016393	0.983607	0	0	0	0	0	0	0.5	2	0	0	0	0	0	0
BH11	0.02	0.04	0.48	0.46	0	0	0	0	2.5	1	1	1	0	0	0	0
BH12	1.000	0.000	0.000	0.000	5.093E-07	0	0	0	1	0	0	0	4.31191E-05	0	0	0
BH13	1.000	0.000	0.000	0.000	5.208E-07	0	0	0	2	0	0	0	4.97231E-05	0	0	0
BH14	1.000	0.000	0.000	0.000	2.951E-06	0	0	0	2	0	0	0	9.75036E-05	0	0	0
BH15	1.000	0.000	0.000	0.000	5.995E-06	0	0	0	2	0	0	0	0.000123457	0	0	0

BH ID	Yield	STRIKE 1	STRIKE 1	YIELD 1	STRIKE 2	STRIKE 2	YIELD 2	STRIKE 3	STRIKE 3	YIELD 3	STRIKE 4	STRIKE 4	YIELD 4
BH1	0.03	54	56	0.03									
BH2	1.11	22	24	0.37	26	28	0.37	32	33	0.37			
BH3	0.06	5	6	0.06									
BH4	2.86	18	18.5	1.43	28.5	30	1.43						
BH5	1.4	22	23	0.2	31	32	1.2						
BH6	0.73	19	20	0.03	26	27	0.1	28.5	29	0.2	32	35	0.4
BH7	0.2	27	28	0.1	33	34	0.1						
BH8	0.3	25	26	0.1	33	35	0.2						
BH9	5.2	26	27	0.2	33	36	5						
BH10	0.61	27.5	28	0.01	36	38	0.6						
BH11	5	34.5	37	0.1	57	58	0.2	61	62	2.4	65	66	2.3
BH12	0.660	26.5	27.5	0.66									
BH13	0.950	19.5	21.0	0.95									
BH14	1.660	29.0	31.0	1.66									
BH15	0.000	50.0	51.0	0.01									

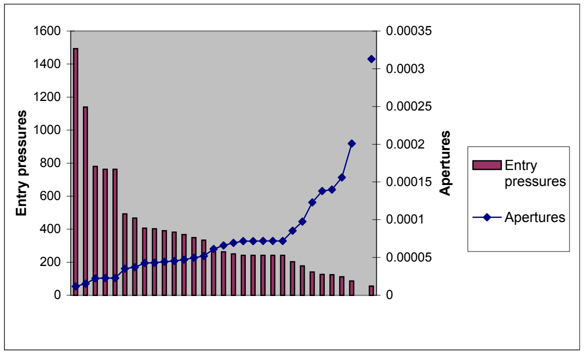
Counter	Aperture, ranked	Entry pressure (e)	Height of DNAPL pool
1	1.16E-05	1493.147	3.658211
2	1.52E-05	1139.507	2.791792
3	2.22E-05	780.2031	1.911498
4	2.27E-05	763.018	1.869394
5	2.27E-05	763.018	1.869394
6	3.52E-05	492.0599	1.205547
7	3.71E-05	466.8601	1.143807
8	4.27E-05	405.6325	0.9938
9	4.31E-05	401.8679	0.984576
10	4.44E-05	390.1015	0.955749
11	4.54E-05	381.509	0.934697
12	4.71E-05	367.739	0.900961
13	4.97E-05	348.5012	0.853828
14	5.20E-05	333.0867	0.816062
15	6.12E-05	283.0148	0.693386
16	6.59E-05	262.8302	0.643934
17	6.93E-05	249.9352	0.612341
18	7.17E-05	241.5692	0.591844
19	7.17E-05	241.5692	0.591844
20	7.18E-05	241.2327	0.59102
21	7.18E-05	241.2327	0.59102
22	7.19E-05	240.8972	0.590198
23	8.55E-05	202.579	0.496319
24	9.75E-05	177.6462	0.435233
25	0.000123	140.8171	0.345002
26	0.000138	125.5109	0.307502
27	0.00014	123.7179	0.303109
28	0.000156	111.0289	0.272021
29	0.000201	86.17168	0.211121
Avg	6.85E-05	3.96E+02	9.71E-01

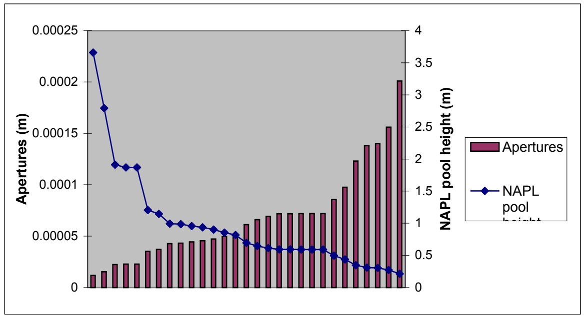
0.01 =s : interfacial tension [N/m]   g = 9.8

30 =q : contact angle [deg]

1000 .=dens h2o (kg/m3)

1080 .=dens napl (kg/m3)   80=diff





APPENDIX E

R&D (ENVIRONMENT AGENCY) RISK WORKSHEETS

R&D Publication 20 Remedial Targets Worksheet, Release 2.2a

Tier 3 - Groundwater

Input Parameters (using pull down menu)

	Variable	Value	Unit	Source
Contaminant		**Acenapthene**		
Target Concentration	C_T	**5.00E-03**	mg/l	

Select analytical solution (click on brown cell below, then on pull-down menu)

Ogata Banks **Equations in R&D Pub. 20**

Enter '1' to simulate vertical dispersion in one direction, '2' for two directions (pull down menu) **2**

Enter '1' if biodegradation rate is for the substance in water,
' if rate is for decay in field conditions (i.e. field data from aquifer) (pull down men **1**

	Variable	Value	Unit	Source of parameter value
Initial contaminant concentration in groundwater at plume core	C_0	3.12E-02	mg/l	*Measured*
Half life for degradation of contaminant in water	$t_{1/2}$	1.14E+02	days	*Howard, 1991*
Calculated decay rate	λ	6.08E-03	$days^{-1}$	
Width of plume in aquifer at source (perpendicular to flow)	Sz	1.00E+02	m	*Measured*
Plume thickness at source	Sy	1.00E+01	m	*Measured*
Saturated aquifer thickness	da	2.00E+01	m	*Measured*
Bulk density of aquifer materials	ρ	1.65E+00	g/cm^3	*Measured*
Effective porosity of aquifer	n	3.00E-02	fraction	*Measured*
Hydraulic gradient	i	4.00E-02	fraction	*Calculated*
Hydraulic conductivity of aquifer	K	3.00E-02	m/d	*Measured*
Distance to compliance point	x	5.00E+01	m	*Measured*
Distance (lateral) to compliance point perpendicular to flow direction	z	0.00E+00	m	*Given*
Distance (depth) to compliance point perpendicular to flow direction	y	0.00E+00	m	*Given*
Time since pollutant entered groundwater	t	9.90E+99	days	*time variant options only*
Parameters values determined from options				
Partition coefficient	Kd	4.90E+00	l/kg	*see options*
Longitudinal dispersivity	ax	2.984	m	*see options*
Transverse dispersivity	az	0.298	m	*see options*
Vertical dispersivity	ay	0.030	m	*see options*

Calculated Parameters

	Variable		
Groundwater flow velocity	v	4.00E-02	m/d
Retardation factor	Rf	2.70E+02	fraction
Decay rate used	λ	2.25E-05	d^{-1}
Rate of contaminant flow due to retardation	u	1.48E-04	m/d
Contaminant concentration at distance x, assuming one-way vertical dispersion	C_{ED}	1.07E-04	mg/l
Contaminant concentration at distance x, assuming two-way vertical dispersion	C_{ED}	1.06E-04	mg/l
Attenuation factor (one way vertical dispersion, C_O/C_{ED})	AF	2.92E+02	
Attenuation factor (two way vertical dispersion, C_O/C_{ED})	AF	2.93E+02	

Remedial Targets

Remedial Target	**LTC3**	**1.47E+00**	**mg/l**
Ogata Banks			

For comparison with measured groundwater concentration.

Distance to compliance point		**50**	**m**	
Concentration of contaminant at compliance point	$C_{ED}/C0$	**1.07E-04**	**mg/l**	Ogata Banks
after		**9.9E+99**	**days**	

Care should be used when calculating remedial targets using the time variant options as this may result in an overestimate of the remedial target.
The recommended value for time when calculating the remedial target is 9.9E+99.

Select Method for deriving Partition Co-efficient (using pull down menu)

Calculate for non-polar organic chemicals

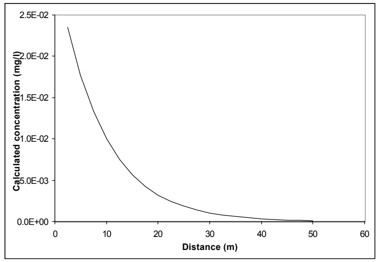
Entry if specify partition coefficient (option)			
Soil water partition coefficient	Kd		l/kg
Entry for non-polar organic chemicals (option)			
Fraction of organic carbon in aquifer	foc	1.00E-03	fraction
Organic carbon partition coefficient	Koc	4.90E+03	l/kg
Entry for ionic organic chemicals (option)			
Sorption coefficient for related species	$K_{oc,n}$		l/kg
Sorption coefficient for ionised species	$K_{oc,i}$		l/kg
pH value	pH		
acid dissociation constant	pKa		
Soil water partition coefficient	Kd	4.90E+00	l/kg

Dispersivity

Calculate dependant on distance to compliance point (0), specify dispersivity (1), or calc after Xu & Eckstein (2) ? **2**

		Enter value	Calc value	Xu & Eckstein	
Longitudinal dispersivity	**ax**	0.00E+00	5.00E+00	2.98E+00	m
Transverse dispersivity	**az**	0.00E+00	5.00E-01	2.98E-01	m
Vertical dispersivity	**ay**	0.00E+00	5.00E-02	2.98E-02	m

For calculated value, assumes ax = 0.1 *x, az = 0.01 * x, ay = 0.001 * x
Xu & Eckstein (1995) report $ax = 0.83(\log_{10}x)^{2.414}$; az = ax/10, ay = ax/100 are assumed



Note graph assumes plume disperses vertically in one direction only. An alternative solution assuming the centre of the plume is located at the mid-depth of the aquifer is presented in the calculation sheets.

This sheet calculates the Tier3 remedial target for groundwater, based on the distance to the receptor or compliance located down hydraulic gradient of the source Three solution methods are included, the preferred option is Ogata

By setting a long travel time it will give the steady state solution, which should be used to calculate remedial targets.

The measured groundwater concentration should be compared with the Tier 3 remedial target to determine the need for further action.

Note if contaminant is not subject to first order degradation, then set half life as 9.0E+99.

Calculated concentrations for distance-concentration graph

Ogata Banks
From calculation sheet

Distance	**Concentration**
	mg/l
2.5	**2.3E-02**
5.0	**1.8E-02**
7.5	**1.3E-02**
10.0	**1.0E-02**
12.5	**7.5E-03**
15.0	**5.7E-03**
17.5	**4.3E-03**
20.0	**3.2E-03**
22.5	**2.4E-03**
25.0	**1.8E-03**
27.5	**1.4E-03**
30.0	**1.0E-03**
32.5	**7.8E-04**
35.0	**5.9E-04**
37.5	**4.4E-04**
40.0	**3.3E-04**
42.5	**2.5E-04**
45.0	**1.9E-04**
47.5	**1.4E-04**
50.0	**1.1E-04**

Site being assessed:	Fictional site
Completed by:	S Hohne
Date:	Enter date
Version:	x.xx

R&D Publication 20 Remedial Targets Worksheet, Release 2.2a

Tier 3 - Groundwater

Input Parameters (using pull down menu)

	Variable	Value	Unit	Source
Contaminant		**Phenol**		
Target Concentration	C_T	**2.00E+00**	mg/l	

Select analytical solution (click on brown cell below, then on pull-down menu)

Ogata Banks **Equations in R&D Pub. 20**

Enter '1' to simulate vertical dispersion in one direction, '2' for two directions (pull down menu)	**2**
Enter '1' if biodegradation rate is for the substance in water, 0' if rate is for decay in field conditions (i.e. field data from aquifer) (pull down men	**1**

	Variable	Value	Unit	Source of parameter value
Initial contaminant concentration in groundwater at plume core	C_0	3.95E+00	mg/l	*Measured*
Half life for degradation of contaminant in water	$t_{1/2}$	3.75E+00	days	*Howard, 1991*
Calculated decay rate	λ	1.85E-01	$days^{-1}$	
Width of plume in aquifer at source (perpendicular to flow)	Sz	1.00E+02	m	*Measured*
Plume thickness at source	Sy	1.00E+01	m	*Measured*
Saturated aquifer thickness	da	2.00E+01	m	*Measured*
Bulk density of aquifer materials	ρ	1.65E+00	g/cm^3	*Measured*
Effective porosity of aquifer	n	3.00E-02	fraction	*Measured*
Hydraulic gradient	i	4.00E-02	fraction	*Calculated*
Hydraulic conductivity of aquifer	K	3.00E-02	m/d	*Measured*
Distance to compliance point	x	5.00E+01	m	*Measured*
Distance (lateral) to compliance point perpendicular to flow direction	z	0.00E+00	m	*Given*
Distance (depth) to compliance point perpendicular to flow direction	y	0.00E+00	m	*Given*
Time since pollutant entered groundwater	t	9.90E+99	days	*time variant options only*
Parameters values determined from options				
Partition coefficient	Kd	2.88E-02	l/kg	*see options*
Longitudinal dispersivity	ax	2.984	m	*see options*
Transverse dispersivity	az	0.298	m	*see options*
Vertical dispersivity	ay	0.030	m	*see options*

Calculated Parameters

	Variable		
Groundwater flow velocity	v	4.00E-02	m/d
Retardation factor	Rf	2.58E+00	fraction
Decay rate used	λ	7.15E-02	d^{-1}
Rate of contaminant flow due to retardation	u	1.55E-02	m/d
Contaminant concentration at distance x, assuming one-way vertical dispersion	C_{ED}	9.27E-24	mg/l
Contaminant concentration at distance x, assuming two-way vertical dispersion	C_{ED}	9.24E-24	mg/l
Attenuation factor (one way vertical dispersion, C_O/C_{ED})	AF	4.26E+23	
Attenuation factor (two way vertical dispersion, C_O/C_{ED})	AF	4.28E+23	

Remedial Targets

Remedial Target	**LTC3**	**8.55E+23**	**mg/l**	For comparison with measured groundwater concentration.
Ogata Banks				
Distance to compliance point		**50**	**m**	
Concentration of contaminant at compliance point	**C_{ED}/C0**	**9.27E-24**	**mg/l**	Ogata Banks
after		**9.9E+99**	**days**	

Care should be used when calculating remedial targets using the time variant options as this may result in an overestimate of the remedial target.
The recommended value for time when calculating the remedial target is 9.9E+99.

Select Method for deriving Partition Co-efficient (using pull down menu)

Calculate for non-polar organic chemicals

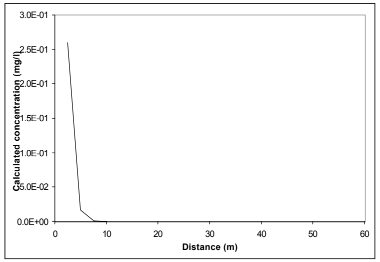
Entry if specify partition coefficient (option)			
Soil water partition coefficient	Kd		l/kg
Entry for non-polar organic chemicals (option)			
Fraction of organic carbon in aquifer	foc	1.00E-03	fraction
Organic carbon partition coefficient	Koc	2.88E+01	l/kg
Entry for ionic organic chemicals (option)			
Sorption coefficient for related species	$K_{oc,n}$		l/kg
Sorption coefficient for ionised species	$K_{oc,i}$		l/kg
pH value	pH		
acid dissociation constant	pKa		
Soil water partition coefficient	Kd	2.88E-02	l/kg

Dispersivity

Calculate dependant on distance to compliance point (0), specify dispersivity (1), or calc after Xu & Eckstein (2) ? **2**

		Enter value	Calc value	Xu & Eckstein	
Longitudinal dispersivity	**ax**	0.00E+00	5.00E+00	2.98E+00	m
Transverse dispersivity	**az**	0.00E+00	5.00E-01	2.98E-01	m
Vertical dispersivity	**ay**	0.00E+00	5.00E-02	2.98E-02	m

For calculated value, assumes ax = 0.1 *x, az = 0.01 * x, ay = 0.001 * x
Xu & Eckstein (1995) report ax = $0.83(\log_{10}x)^{2.414}$; az = ax/10, ay = ax/100 are assumed



Note graph assumes plume disperses vertically in one direction only. An alternative solution assuming the centre of the plume is located at the mid-depth of the aquifer is presented in the calculation sheets.

This sheet calculates the Tier3 remedial target for groundwater, based on the distance to the receptor or compliance located down hydraulic gradient of the source Three solution methods are included, the preferred option is Ogata

By setting a long travel time it will give the steady state solution, which should be used to calculate remedial targets.

The measured groundwater concentration should be compared
with the Tier 3 remedial target to determine the need for further action.
Note if contaminant is not subject to first order degradation, then set half life as 9.0E+99.

Calculated concentrations for distance-concentration graph

Ogata Banks
From calculation sheet

Distance	**Concentration**
	mg/l
2.5	**2.6E-01**
5.0	**1.7E-02**
7.5	**1.1E-03**
10.0	**7.4E-05**
12.5	**4.9E-06**
15.0	**3.2E-07**
17.5	**2.1E-08**
20.0	**1.4E-09**
22.5	**9.2E-11**
25.0	**6.1E-12**
27.5	**4.0E-13**
30.0	**2.6E-14**
32.5	**1.7E-15**
35.0	**1.1E-16**
37.5	**7.5E-18**
40.0	**4.9E-19**
42.5	**3.2E-20**
45.0	**2.1E-21**
47.5	**1.4E-22**
50.0	**9.3E-24**

Site being assessed: Fictional site
Completed by: S Hohne
Date: Enter date
Version: x.xx

R&D Publication 20 Remedial Targets Worksheet, Release 2.2a

Tier 3 - Groundwater

Input Parameters (using pull down menu)

	Variable	Value	Unit	Source
Contaminant		**Phenanthrene**		
Target Concentration	C_T	**5.00E-03**	mg/l	

Select analytical solution (click on brown cell below, then on pull-down menu)

Ogata Banks **Equations in R&D Pub. 20**

Enter '1' to simulate vertical dispersion in one direction, '2' for two directions (pull down menu) **2**

Enter '1' if biodegradation rate is for the substance in water,
)' if rate is for decay in field conditions (i.e. field data from aquifer) (pull down menu **1**

	Variable	Value	Unit	Source of parameter value
Initial contaminant concentration in groundwater at plume core	C_0	3.12E-02	mg/l	*Measured*
Half life for degradation of contaminant in water	$t_{1/2}$	2.16E+02	days	*Howard, 1991*
Calculated decay rate	λ	3.21E-03	$days^{-1}$	
Width of plume in aquifer at source (perpendicular to flow)	Sz	1.00E+02	m	*Measured*
Plume thickness at source	Sy	1.00E+01	m	*Measured*
Saturated aquifer thickness	da	2.00E+01	m	*Measured*
Bulk density of aquifer materials	ρ	1.65E+00	g/cm^3	*Measured*
Effective porosity of aquifer	n	3.00E-02	fraction	*Measured*
Hydraulic gradient	i	4.00E-02	fraction	*Calculated*
Hydraulic conductivity of aquifer	K	3.00E-02	m/d	*Measured*
Distance to compliance point	x	5.00E+01	m	*Measured*
Distance (lateral) to compliance point perpendicular to flow direction	z	0.00E+00	m	*Given*
Distance (depth) to compliance point perpendicular to flow direction	y	0.00E+00	m	*Given*
Time since pollutant entered groundwater	t	9.90E+99	days	*time variant options only*
Parameters values determined from options				
Partition coefficient	Kd	1.13E+01	l/kg	*see options*
Longitudinal dispersivity	ax	2.984	m	*see options*
Transverse dispersivity	az	0.298	m	*see options*
Vertical dispersivity	ay	0.030	m	*see options*

Calculated Parameters

	Variable		
Groundwater flow velocity	v	4.00E-02	m/d
Retardation factor	Rf	6.20E+02	fraction
Decay rate used	λ	5.17E-06	d^{-1}
Rate of contaminant flow due to retardation	u	6.45E-05	m/d
Contaminant concentration at distance x, assuming one-way vertical dispersion	C_{ED}	1.10E-03	mg/l
Contaminant concentration at distance x, assuming two-way vertical dispersion	C_{ED}	1.10E-03	mg/l
Attenuation factor (one way vertical dispersion, C_O/C_{ED})	AF	2.83E+01	
Attenuation factor (two way vertical dispersion, C_O/C_{ED})	AF	2.84E+01	

Remedial Targets

Remedial Target	**LTC3**	**1.42E-01**	**mg/l**	For comparison with measured groundwater concentration.
Ogata Banks				
Distance to compliance point		**50**	**m**	
Concentration of contaminant at compliance point	**$C_{ED}/C0$**	**1.10E-03**	**mg/l**	Ogata Banks
after		**9.9E+99**	**days**	

Care should be used when calculating remedial targets using the time variant options as this may result in an overestimate of the remedial target.
The recommended value for time when calculating the remedial target is 9.9E+99.

Select Method for deriving Partition Co-efficient (using pull down menu)

Calculate for non-polar organic chemicals

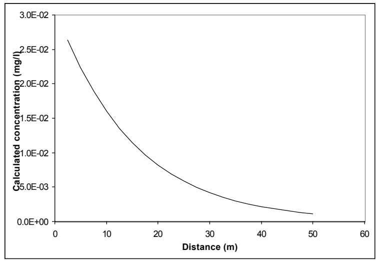
Entry if specify partition coefficient (option)			
Soil water partition coefficient	Kd		l/kg
Entry for non-polar organic chemicals (option)			
Fraction of organic carbon in aquifer	foc	1.00E-03	fraction
Organic carbon partition coefficient	Koc	1.13E+04	l/kg
Entry for ionic organic chemicals (option)			
Sorption coefficient for related species	$K_{oc,n}$		l/kg
Sorption coefficient for ionised species	$K_{oc,i}$		l/kg
pH value	pH		
acid dissociation constant	pKa		
Soil water partition coefficient	Kd	1.13E+01	l/kg

Dispersivity

Calculate dependant on distance to compliance point (0), specify dispersivity (1), or calc after Xu & Eckstein (2) ? **2**

		Enter value	Calc value	Xu & Eckstein	
Longitudinal dispersivity	**ax**	0.00E+00	5.00E+00	2.98E+00	m
Transverse dispersivity	**az**	0.00E+00	5.00E-01	2.98E-01	m
Vertical dispersivity	**ay**	0.00E+00	5.00E-02	2.98E-02	m

For calculated value, assumes ax = 0.1 *x, az = 0.01 * x, ay = 0.001 * x
Xu & Eckstein (1995) report $ax = 0.83(\log_{10}x)^{2.414}$; az = ax/10, ay = ax/100 are assumed



Note graph assumes plume disperses vertically in one direction only. An alternative solution assuming the centre of the plume is located at the mid-depth of the aquifer is presented in the calculation sheets.

This sheet calculates the Tier3 remedial target for groundwater, based on the distance to the receptor or compliance located down hydraulic gradient of the source Three solution methods are included, the preferred option is Ogata Banks.

By setting a long travel time it will give the steady state solution, which should be used to calculate remedial targets.

The measured groundwater concentration should be compared
with the Tier 3 remedial target to determine the need for further action.
Note if contaminant is not subject to first order degradation, then set half life as 9.0E+99.

Calculated concentrations for distance-concentration graph

Ogata Banks
From calculation sheet

Distance	**Concentration**
	mg/l
2.5	**2.6E-02**
5.0	**2.2E-02**
7.5	**1.9E-02**
10.0	**1.6E-02**
12.5	**1.4E-02**
15.0	**1.1E-02**
17.5	**9.7E-03**
20.0	**8.2E-03**
22.5	**6.9E-03**
25.0	**5.9E-03**
27.5	**5.0E-03**
30.0	**4.2E-03**
32.5	**3.5E-03**
35.0	**3.0E-03**
37.5	**2.5E-03**
40.0	**2.1E-03**
42.5	**1.8E-03**
45.0	**1.5E-03**
47.5	**1.3E-03**
50.0	**1.1E-03**

Site being assessed:	Fictional site
Completed by:	S Hohne
Date:	Enter date
Version:	x.xx

R&D Publication 20 Remedial Targets Worksheet, Release 2.2a

Tier 3 - Groundwater

Input Parameters (using pull down menu)

	Variable	Value	Unit	Source
Contaminant		Napthalene		
Target Concentration	C_T	**7.00E-02**	mg/l	

Select analytical solution (click on brown cell below, then on pull-down menu)

Ogata Banks — **Equations in R&D Pub. 20**

Enter '1' to simulate vertical dispersion in one direction, '2' for two directions (pull down menu) **2**

Enter '1' if biodegradation rate is for the substance in water,
)' if rate is for decay in field conditions (i.e. field data from aquifer) (pull down men **1**

	Variable	Value	Unit	Source of parameter value
Initial contaminant concentration in groundwater at plume core	C_0	3.60E+01	mg/l	*Measured*
Half life for degradation of contaminant in water	$t_{1/2}$	1.30E+02	days	*Howard, 1991*
Calculated decay rate	λ	5.33E-03	days^{-1}	
Width of plume in aquifer at source (perpendicular to flow)	Sz	1.00E+02	m	*Measured*
Plume thickness at source	Sy	1.00E+01	m	*Measured*
Saturated aquifer thickness	da	2.00E+01	m	*Measured*
Bulk density of aquifer materials	ρ	1.65E+00	g/cm^3	*Measured*
Effective porosity of aquifer	n	3.00E-02	fraction	*Measured*
Hydraulic gradient	i	4.00E-02	fraction	*Calculated*
Hydraulic conductivity of aquifer	K	3.00E-02	m/d	*Measured*
Distance to compliance point	x	5.00E+01	m	*Measured*
Distance (lateral) to compliance point perpendicular to flow direction	z	0.00E+00	m	*Given*
Distance (depth) to compliance point perpendicular to flow direction	y	0.00E+00	m	*Given*
Time since pollutant entered groundwater	t	9.90E+99	days	*time variant options only*
Parameters values determined from options				
Partition coefficient	Kd	1.19E+00	l/kg	*see options*
Longitudinal dispersivity	ax	2.984	m	*see options*
Transverse dispersivity	az	0.298	m	*see options*
Vertical dispersivity	ay	0.030	m	*see options*

Calculated Parameters

	Variable		
Groundwater flow velocity	v	4.00E-02	m/d
Retardation factor	Rf	6.65E+01	fraction
Decay rate used	λ	8.02E-05	d^{-1}
Rate of contaminant flow due to retardation	u	6.01E-04	m/d
Contaminant concentration at distance x, assuming one-way vertical dispersion	C_{ED}	2.18E-01	mg/l
Contaminant concentration at distance x, assuming two-way vertical dispersion	C_{ED}	2.17E-01	mg/l
Attenuation factor (one way vertical dispersion, C_O/C_{ED})	AF	1.65E+02	
Attenuation factor (two way vertical dispersion, C_O/C_{ED})	AF	1.66E+02	

Remedial Targets

Remedial Target	**LTC3**	**1.16E+01**	**mg/l**	For comparison with measured groundwater concentration.
Ogata Banks				
Distance to compliance point		**50**	**m**	
Concentration of contaminant at compliance point	**C_{ED}/C0**	**2.18E-01**	**mg/l**	Ogata Banks
after		**9.9E+99**	**days**	

Care should be used when calculating remedial targets using the time variant options as this may result in an overestimate of the remedial target.
The recommended value for time when calculating the remedial target is 9.9E+99.

Select Method for deriving Partition Co-efficient (using pull down menu)

Calculate for non-polar organic chemicals

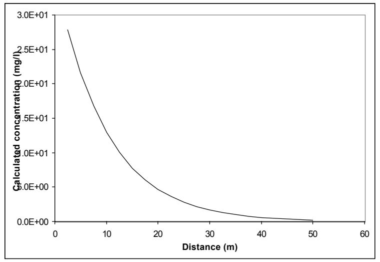
Entry if specify partition coefficient (option)			
Soil water partition coefficient	Kd		l/kg
Entry for non-polar organic chemicals (option)			
Fraction of organic carbon in aquifer	foc	1.00E-03	fraction
Organic carbon partition coefficient	Koc	1.19E+03	l/kg
Entry for ionic organic chemicals (option)			
Sorption coefficient for related species	$K_{oc,n}$		l/kg
Sorption coefficient for ionised species	$K_{oc,i}$		l/kg
pH value	pH		
acid dissociation constant	pKa		
Soil water partition coefficient	Kd	1.19E+00	l/kg

Dispersivity

Calculate dependant on distance to compliance point (0), specify dispersivity (1), or calc after Xu & Eckstein (2) ? **2**

		Enter value	Calc value	Xu & Eckstein	
Longitudinal dispersivity	**ax**	0.00E+00	5.00E+00	2.98E+00	m
Transverse dispersivity	**az**	0.00E+00	5.00E-01	2.98E-01	m
Vertical dispersivity	**ay**	0.00E+00	5.00E-02	2.98E-02	m

For calculated value, assumes ax = 0.1 *x, az = 0.01 * x, ay = 0.001 * x
Xu & Eckstein (1995) report ax = $0.83(\log_{10}x)^{2.414}$; az = ax/10, ay = ax/100 are assumed



Note graph assumes plume disperses vertically in one direction only. An alternative solution assuming the centre of the plume is located at the mid-depth of the aquifer is presented in the calculation sheets.

This sheet calculates the Tier3 remedial target for groundwater, based on the distance to the receptor or compliance located down hydraulic gradient of the source Three solution methods are included, the preferred option is Ogata

By setting a long travel time it will give the steady state solution, which should be used to calculate remedial targets.

The measured groundwater concentration should be compared
with the Tier 3 remedial target to determine the need for further action.
Note if contaminant is not subject to first order degradation, then set half life as 9.0E+99.

Site being assessed:	Fictional site
Completed by:	S Hohne
Date:	Enter date
Version:	x.xx

Calculated concentrations for distance-concentration graph

Ogata Banks
From calculation sheet

Distance	**Concentration**
	mg/l
2.5	**2.8E+01**
5.0	**2.2E+01**
7.5	**1.7E+01**
10.0	**1.3E+01**
12.5	**1.0E+01**
15.0	**7.8E+00**
17.5	**6.0E+00**
20.0	**4.7E+00**
22.5	**3.6E+00**
25.0	**2.8E+00**
27.5	**2.2E+00**
30.0	**1.7E+00**
32.5	**1.3E+00**
35.0	**1.0E+00**
37.5	**7.8E-01**
40.0	**6.0E-01**
42.5	**4.7E-01**
45.0	**3.6E-01**
47.5	**2.8E-01**
50.0	**2.2E-01**

R&D Publication 20 Remedial Targets Worksheet, Release 2.2a

Tier 3 - Groundwater

ENVIRONMENT AGENCY

Input Parameters (using pull down menu)

Input Parameters (using pull down menu)	Variable	Value	Unit	Source
Contaminant		**M-xylene**		
Target Concentration	C_T	**7.00E-02**	mg/l	

Select analytical solution (click on brown cell below, then on pull-down menu)

Ogata Banks **Equations in R&D Pub. 20**

Enter '1' to simulate vertical dispersion in one direction, '2' for two directions (pull down menu) **2**

Enter '1' if biodegradation rate is for the substance in water,
' if rate is for decay in field conditions (i.e. field data from aquifer) (pull down men **1**

	Variable	Value	Unit	Source of parameter value
Initial contaminant concentration in groundwater at plume core	C_0	8.50E-01	mg/l	*Measured*
Half life for degradation of contaminant in water	$t_{1/2}$	1.87E+02	days	*Howard, 1991*
Calculated decay rate	λ	3.71E-03	$days^{-1}$	
Width of plume in aquifer at source (perpendicular to flow)	Sz	1.00E+02	m	*Measured*
Plume thickness at source	Sy	1.00E+01	m	*Measured*
Saturated aquifer thickness	da	2.00E+01	m	*Measured*
Bulk density of aquifer materials	ρ	1.65E+00	g/cm^3	*Measured*
Effective porosity of aquifer	n	3.00E-02	fraction	*Measured*
Hydraulic gradient	i	4.00E-02	fraction	*Calculated*
Hydraulic conductivity of aquifer	K	3.00E-02	m/d	*Measured*
Distance to compliance point	x	5.00E+01	m	*Measured*
Distance (lateral) to compliance point perpendicular to flow direction	z	0.00E+00	m	*Given*
Distance (depth) to compliance point perpendicular to flow direction	y	0.00E+00	m	*Given*
Time since pollutant entered groundwater	t	9.90E+99	days	*time variant options only*
Parameters values determined from options				
Partition coefficient	Kd	1.29E-01	l/kg	*see options*
Longitudinal dispersivity	ax	2.984	m	*see options*
Transverse dispersivity	az	0.298	m	*see options*
Vertical dispersivity	ay	0.030	m	*see options*

Calculated Parameters

Calculated Parameters	Variable		
Groundwater flow velocity	v	4.00E-02	m/d
Retardation factor	Rf	8.10E+00	fraction
Decay rate used	λ	4.58E-04	d^{-1}
Rate of contaminant flow due to retardation	u	4.94E-03	m/d
Contaminant concentration at distance x, assuming one-way vertical dispersion	C_{ED}	1.94E-02	mg/l
Contaminant concentration at distance x, assuming two-way vertical dispersion	C_{ED}	1.93E-02	mg/l
Attenuation factor (one way vertical dispersion, C_O/C_{ED})	AF	4.38E+01	
Attenuation factor (two way vertical dispersion, C_O/C_{ED})	AF	4.40E+01	

Remedial Targets

Remedial Target	**LTC3**	**3.08E+00**	**mg/l**	For comparison with measured groundwater concentration.
Ogata Banks				
Distance to compliance point		**50**	**m**	
Concentration of contaminant at compliance point	$C_{ED}/C0$	**1.94E-02**	**mg/l**	Ogata Banks
after		**9.9E+99**	**days**	

Care should be used when calculating remedial targets using the time variant options as this may result in an overestimate of the remedial target.
The recommended value for time when calculating the remedial target is 9.9E+99.

Select Method for deriving Partition Co-efficient (using pull down menu)

Calculate for non-polar organic chemicals

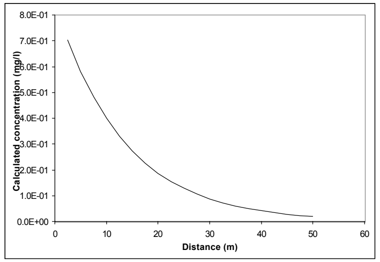
Entry if specify partition coefficient (option)			
Soil water partition coefficient	Kd		l/kg
Entry for non-polar organic chemicals (option)			
Fraction of organic carbon in aquifer	foc	1.00E-03	fraction
Organic carbon partition coefficient	Koc	1.29E+02	l/kg
Entry for ionic organic chemicals (option)			
Sorption coefficient for related species	$K_{oc,n}$		l/kg
Sorption coefficient for ionised species	$K_{oc,i}$		l/kg
pH value	pH		
acid dissociation constant	pKa		
Soil water partition coefficient	Kd	1.29E-01	l/kg

Dispersivity

Calculate dependant on distance to compliance point (0), specify dispersivity (1), or calc after Xu & Eckstein (2) ? **2**

		Enter value	Calc value	Xu & Eckstein	
Longitudinal dispersivity	**ax**	0.00E+00	5.00E+00	2.98E+00	m
Transverse dispersivity	**az**	0.00E+00	5.00E-01	2.98E-01	m
Vertical dispersivity	**ay**	0.00E+00	5.00E-02	2.98E-02	m

For calculated value, assumes ax = 0.1 *x, az = 0.01 * x, ay = 0.001 * x
Xu & Eckstein (1995) report ax = $0.83(\log_{10}x)^{2.414}$; az = ax/10, ay = ax/100 are assumed



Note graph assumes plume disperses vertically in one direction only. An alternative solution assuming the centre of the plume is located at the mid-depth of the aquifer is presented in the calculation sheets.

This sheet calculates the Tier3 remedial target for groundwater, based on the distance to the receptor or compliance located down hydraulic gradient of the source Three solution methods are included, the preferred option is Ogata

By setting a long travel time it will give the steady state solution, which should be used to calculate remedial targets.

The measured groundwater concentration should be compared with the Tier 3 remedial target to determine the need for further action.
Note if contaminant is not subject to first order degradation, then set half life as 9.0E+99.

Calculated concentrations for distance-concentration graph

Ogata Banks
From calculation sheet

Distance	**Concentration** **mg/l**
2.5	**7.0E-01**
5.0	**5.8E-01**
7.5	**4.8E-01**
10.0	**4.0E-01**
12.5	**3.3E-01**
15.0	**2.7E-01**
17.5	**2.3E-01**
20.0	**1.9E-01**
22.5	**1.6E-01**
25.0	**1.3E-01**
27.5	**1.1E-01**
30.0	**8.8E-02**
32.5	**7.3E-02**
35.0	**6.0E-02**
37.5	**5.0E-02**
40.0	**4.1E-02**
42.5	**3.4E-02**
45.0	**2.8E-02**
47.5	**2.3E-02**
50.0	**1.9E-02**

Site being assessed:	Fictional site
Completed by:	S Hohne
Date:	Enter date
Version:	x.xx

R&D Publication 20 Remedial Targets Worksheet, Release 2.2a

ENVIRONMENT AGENCY

Tier 3 - Groundwater

Input Parameters (using pull down menu)

Input Parameters (using pull down menu)	Variable	Value	Unit	Source
Contaminant		**Fluoranthene**		
Target Concentration	C_T	**1.00E-03**	mg/l	

Select analytical solution (click on brown cell below, then on pull-down menu)

Ogata Banks **Equations in R&D Pub. 20**

Enter '1' to simulate vertical dispersion in one direction, '2' for two directions (pull down menu) **1**

Enter '1' if biodegradation rate is for the substance in water,
' if rate is for decay in field conditions (i.e. field data from aquifer) (pull down men **1**

				Source of parameter value
Initial contaminant concentration in groundwater at plume core	C_0	1.40E-02	mg/l	*Measured*
Half life for degradation of contaminant in water	$t_{1/2}$	5.80E+02	days	*Howard, 1991*
Calculated decay rate	λ	1.20E-03	days^{-1}	
Width of plume in aquifer at source (perpendicular to flow)	Sz	1.00E+02	m	*Measured*
Plume thickness at source	Sy	1.00E+01	m	*Measured*
Saturated aquifer thickness	da	2.00E+01	m	*Measured*
Bulk density of aquifer materials	ρ	1.65E+00	g/cm^3	*Measured*
Effective porosity of aquifer	n	3.00E-02	fraction	*Measured*
Hydraulic gradient	i	4.00E-02	fraction	*Calculated*
Hydraulic conductivity of aquifer	K	3.00E-02	m/d	*Measured*
Distance to compliance point	x	5.00E+01	m	*Measured*
Distance (lateral) to compliance point perpendicular to flow direction	z	0.00E+00	m	*Given*
Distance (depth) to compliance point perpendicular to flow direction	y	0.00E+00	m	*Given*
Time since pollutant entered groundwater	t	9.90E+99	days	*time variant options only*
Parameters values determined from options				
Partition coefficient	Kd	4.91E+01	l/kg	*see options*
Longitudinal dispersivity	ax	2.984	m	*see options*
Transverse dispersivity	az	0.298	m	*see options*
Vertical dispersivity	ay	0.030	m	*see options*

Calculated Parameters

Calculated Parameters	Variable		
Groundwater flow velocity	v	4.00E-02	m/d
Retardation factor	Rf	2.70E+03	fraction
Decay rate used	λ	4.42E-07	d^{-1}
Rate of contaminant flow due to retardation	u	1.48E-05	m/d
Contaminant concentration at distance x, assuming one-way vertical dispersion	C_{ED}	3.52E-03	mg/l
Contaminant concentration at distance x, assuming two-way vertical dispersion	C_{ED}	3.51E-03	mg/l
Attenuation factor (one way vertical dispersion, C_O/C_{ED})	AF	3.98E+00	
Attenuation factor (two way vertical dispersion, C_O/C_{ED})	AF	3.99E+00	

Remedial Targets

Remedial Target	**LTC3**	**3.98E-03**	**mg/l**	For comparison with measured groundwater concentration.
Ogata Banks				
Distance to compliance point		**50**	**m**	
Concentration of contaminant at compliance point	**C_{ED}/C0**	**3.52E-03**	**mg/l**	Ogata Banks
after		**9.9E+99**	**days**	

Care should be used when calculating remedial targets using the time variant options as this may result in an overestimate of the remedial target.
The recommended value for time when calculating the remedial target is 9.9E+99.

Select Method for deriving Partition Co-efficient (using pull down menu)

Calculate for non-polar organic chemicals

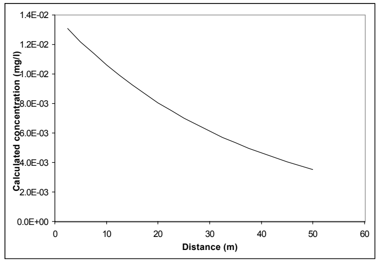
Entry if specify partition coefficient (option)			
Soil water partition coefficient	Kd		l/kg
Entry for non-polar organic chemicals (option)			
Fraction of organic carbon in aquifer	foc	1.00E-03	fraction
Organic carbon partition coefficient	Koc	4.91E+04	l/kg
Entry for ionic organic chemicals (option)			
Sorption coefficient for related species	$K_{oc,n}$		l/kg
Sorption coefficient for ionised species	$K_{oc,i}$		l/kg
pH value	pH		
acid dissociation constant	pKa		
Soil water partition coefficient	Kd	4.91E+01	l/kg

Dispersivity

Calculate dependant on distance to compliance point (0), **2**
specify dispersivity (1), or calc after Xu & Eckstein (2) ?

		Enter value	Calc value	Xu & Eckstein	
Longitudinal dispersivity	**ax**	0.00E+00	5.00E+00	2.98E+00	m
Transverse dispersivity	**az**	0.00E+00	5.00E-01	2.98E-01	m
Vertical dispersivity	**ay**	0.00E+00	5.00E-02	2.98E-02	m

For calculated value, assumes ax = 0.1 *x, az = 0.01 * x, ay = 0.001 * x
Xu & Eckstein (1995) report ax = $0.83(\log_{10}x)^{2.414}$; az = ax/10, ay = ax/100 are assumed



Note graph assumes plume disperses vertically in one direction only. An alternative solution assuming the centre of the plume is located at the mid-depth of the aquifer is presented in the calculation sheets.

This sheet calculates the Tier3 remedial target for groundwater, based on the distance to the receptor or compliance located down hydraulic gradient of the source Three solution methods are included, the preferred option is Ogata

By setting a long travel time it will give the steady state solution, which should be used to calculate remedial targets.

The measured groundwater concentration should be compared
with the Tier 3 remedial target to determine the need for further action.
Note if contaminant is not subject to first order degradation, then set half life as 9.0E+99.

Site being assessed:	Fictional site
Completed by:	S Hohne
Date:	Enter date
Version:	x.xx

Calculated concentrations for distance-concentration graph

Ogata Banks
From calculation sheet

Distance	Concentration
	mg/l
2.5	1.3E-02
5.0	1.2E-02
7.5	1.1E-02
10.0	1.1E-02
12.5	9.9E-03
15.0	9.3E-03
17.5	8.6E-03
20.0	8.1E-03
22.5	7.5E-03
25.0	7.0E-03
27.5	6.6E-03
30.0	6.1E-03
32.5	5.7E-03
35.0	5.3E-03
37.5	5.0E-03
40.0	4.6E-03
42.5	4.3E-03
45.0	4.0E-03
47.5	3.8E-03
50.0	3.5E-03

R&D Publication 20 Remedial Targets Worksheet, Release 2.2a

Tier 3 - Groundwater

ENVIRONMENT AGENCY

Input Parameters (using pull down menu)

	Variable	Value	Unit	Source
Contaminant		Ethylbenzene		
Target Concentration	C_T	**1.50E-02**	mg/l	

Select analytical solution (click on brown cell below, then on pull-down menu)

Ogata Banks — **Equations in R&D Pub. 20**

Enter '1' to simulate vertical dispersion in one direction, '2' for two directions (pull down menu) **2**

Enter '1' if biodegradation rate is for the substance in water,
' if rate is for decay in field conditions (i.e. field data from aquifer) (pull down men **1**

	Variable	Value	Unit	Source of parameter value
Initial contaminant concentration in groundwater at plume core	C_0	2.38E-01	mg/l	*Measured*
Half life for degradation of contaminant in water	$t_{1/2}$	1.73E+02	days	*Howard, 1991; Thierrin, 1995*
Calculated decay rate	λ	4.01E-03	days^{-1}	
Width of plume in aquifer at source (perpendicular to flow)	Sz	1.00E+02	m	*Measured*
Plume thickness at source	Sy	1.00E+01	m	*Measured*
Saturated aquifer thickness	da	2.00E+01	m	*Measured*
Bulk density of aquifer materials	ρ	1.65E+00	g/cm^3	*Measured*
Effective porosity of aquifer	n	3.00E-02	fraction	*Measured*
Hydraulic gradient	i	4.00E-02	fraction	*Calculated*
Hydraulic conductivity of aquifer	K	3.00E-02	m/d	*Measured*
Distance to compliance point	x	5.00E+01	m	*Measured*
Distance (lateral) to compliance point perpendicular to flow direction	z	0.00E+00	m	*Given*
Distance (depth) to compliance point perpendicular to flow direction	y	0.00E+00	m	*Given*
Time since pollutant entered groundwater	t	9.90E+99	days	*time variant options only*
Parameters values determined from options				
Partition coefficient	Kd	2.04E-01	l/kg	*see options*
Longitudinal dispersivity	ax	2.984	m	*see options*
Transverse dispersivity	az	0.298	m	*see options*
Vertical dispersivity	ay	0.030	m	*see options*

Calculated Parameters

	Variable		
Groundwater flow velocity	v	4.00E-02	m/d
Retardation factor	Rf	1.22E+01	fraction
Decay rate used	λ	3.28E-04	d^{-1}
Rate of contaminant flow due to retardation	u	3.27E-03	m/d
Contaminant concentration at distance x, assuming one-way vertical dispersion	C_{ED}	4.20E-03	mg/l
Contaminant concentration at distance x, assuming two-way vertical dispersion	C_{ED}	4.19E-03	mg/l
Attenuation factor (one way vertical dispersion, C_O/C_{ED})	AF	5.66E+01	
Attenuation factor (two way vertical dispersion, C_O/C_{ED})	AF	5.68E+01	

Remedial Targets

Remedial Target	**LTC3**	**8.52E-01**	**mg/l**
Ogata Banks			

For comparison with measured groundwater concentration.

Distance to compliance point **50** **m**

Concentration of contaminant at compliance point **C_{ED}/C0** **4.20E-03** **mg/l** Ogata Banks
after **9.9E+99** **days**

Care should be used when calculating remedial targets using the time variant options as this may result in an overestimate of the remedial target.
The recommended value for time when calculating the remedial target is 9.9E+99.

Select Method for deriving Partition Co-efficient (using pull down menu)

Calculate for non-polar organic chemicals

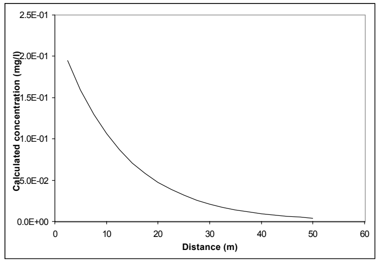
Entry if specify partition coefficient (option)			
Soil water partition coefficient	Kd		l/kg
Entry for non-polar organic chemicals (option)			
Fraction of organic carbon in aquifer	foc	1.00E-03	fraction
Organic carbon partition coefficient	Koc	2.04E+02	l/kg
Entry for ionic organic chemicals (option)			
Sorption coefficient for related species	$K_{oc,n}$		l/kg
Sorption coefficient for ionised species	$K_{oc,i}$		l/kg
pH value	pH		
acid dissociation constant	pKa		
Soil water partition coefficient	Kd	2.04E-01	l/kg

Dispersivity

Calculate dependant on distance to compliance point (0), specify dispersivity (1), or calc after Xu & Eckstein (2) ? **2**

		Enter value	Calc value	Xu & Eckstein	
Longitudinal dispersivity	**ax**	0.00E+00	5.00E+00	2.98E+00	m
Transverse dispersivity	**az**	0.00E+00	5.00E-01	2.98E-01	m
Vertical dispersivity	**ay**	0.00E+00	5.00E-02	2.98E-02	m

For calculated value, assumes ax = 0.1 *x, az = 0.01 * x, ay = 0.001 * x
Xu & Eckstein (1995) report ax = $0.83(\log_{10}x)^{2.414}$; az = ax/10, ay = ax/100 are assumed



Note graph assumes plume disperses vertically in one direction only. An alternative solution assuming the centre of the plume is located at the mid-depth of the aquifer is presented in the calculation sheets.

This sheet calculates the Tier3 remedial target for groundwater, based on the distance to the receptor or compliance located down hydraulic gradient of the source Three solution methods are included, the preferred option is Ogata

By setting a long travel time it will give the steady state solution, which should be used to calculate remedial targets.

The measured groundwater concentration should be compared
with the Tier 3 remedial target to determine the need for further action.
Note if contaminant is not subject to first order degradation, then set half life as 9.0E+99.

Calculated concentrations for distance-concentration graph

Ogata Banks
From calculation sheet

Distance	**Concentration**
	mg/l
2.5	**1.9E-01**
5.0	**1.6E-01**
7.5	**1.3E-01**
10.0	**1.1E-01**
12.5	**8.7E-02**
15.0	**7.1E-02**
17.5	**5.8E-02**
20.0	**4.7E-02**
22.5	**3.9E-02**
25.0	**3.2E-02**
27.5	**2.6E-02**
30.0	**2.1E-02**
32.5	**1.7E-02**
35.0	**1.4E-02**
37.5	**1.2E-02**
40.0	**9.4E-03**
42.5	**7.7E-03**
45.0	**6.3E-03**
47.5	**5.1E-03**
50.0	**4.2E-03**

Site being assessed:	Fictional site
Completed by:	S Hohne
Date:	Enter date
Version:	x.xx

R&D Publication 20 Remedial Targets Worksheet, Release 2.2a

Tier 3 - Groundwater

Input Parameters (using pull down menu)

Input Parameters	Variable	Value	Unit	Source
Contaminant		**Chloroform**		
Target Concentration	C_T	**8.00E-02**	mg/l	

Select analytical solution (click on brown cell below, then on pull-down menu)

Ogata Banks — **Equations in R&D Pub. 20**

Enter '1' to simulate vertical dispersion in one direction, '2' for two directions (pull down menu)	**2**
Enter '1' if biodegradation rate is for the substance in water,)' if rate is for decay in field conditions (i.e. field data from aquifer) (pull down men	**1**

Parameter	Variable	Value	Unit	Source of parameter value
Initial contaminant concentration in groundwater at plume core	C_0	1.33E+00	mg/l	*Measured*
Half life for degradation of contaminant in water	$t_{1/2}$	9.28E+02	days	*Howard, 1991*
Calculated decay rate	λ	7.47E-04	$days^{-1}$	
Width of plume in aquifer at source (perpendicular to flow)	Sz	1.00E+02	m	*Measured*
Plume thickness at source	Sy	1.00E+01	m	*Measured*
Saturated aquifer thickness	da	2.00E+01	m	*Measured*
Bulk density of aquifer materials	ρ	1.65E+00	g/cm^3	*Measured*
Effective porosity of aquifer	n	3.00E-02	fraction	*Measured*
Hydraulic gradient	i	4.00E-02	fraction	*Calculated*
Hydraulic conductivity of aquifer	K	3.00E-02	m/d	*Measured*
Distance to compliance point	x	5.00E+01	m	*Measured*
Distance (lateral) to compliance point perpendicular to flow direction	z	0.00E+00	m	*Given*
Distance (depth) to compliance point perpendicular to flow direction	y	0.00E+00	m	*Given*
Time since pollutant entered groundwater	t	9.90E+99	days	*time variant options only*
Parameters values determined from options				
Partition coefficient	Kd	5.25E-02	l/kg	*see options*
Longitudinal dispersivity	ax	2.984	m	*see options*
Transverse dispersivity	az	0.298	m	*see options*
Vertical dispersivity	ay	0.030	m	*see options*

Calculated Parameters

Calculated Parameters	Variable	Value	Unit
Groundwater flow velocity	v	4.00E-02	m/d
Retardation factor	Rf	3.89E+00	fraction
Decay rate used	λ	1.92E-04	d^{-1}
Rate of contaminant flow due to retardation	u	1.03E-02	m/d
Contaminant concentration at distance x, assuming one-way vertical dispersion	C_{ED}	5.46E-01	mg/l
Contaminant concentration at distance x, assuming two-way vertical dispersion	C_{ED}	5.44E-01	mg/l
Attenuation factor (one way vertical dispersion, C_O/C_{ED})	AF	2.43E+00	
Attenuation factor (two way vertical dispersion, C_O/C_{ED})	AF	2.44E+00	

Remedial Targets

Remedial Target	**LTC3**	**1.95E-01**	**mg/l**	For comparison with measured groundwater concentration.
Ogata Banks				
Distance to compliance point		**50**	**m**	
Concentration of contaminant at compliance point	$C_{ED}/C0$	**5.46E-01**	**mg/l**	Ogata Banks
after		**9.9E+99**	**days**	

Care should be used when calculating remedial targets using the time variant options as this may result in an overestimate of the remedial target.
The recommended value for time when calculating the remedial target is 9.9E+99.

Select Method for deriving Partition Co-efficient (using pull down menu)

Calculate for non-polar organic chemicals

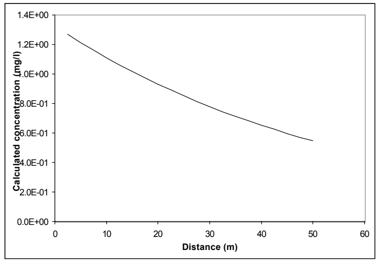
Entry if specify partition coefficient (option)			
Soil water partition coefficient	Kd		l/kg
Entry for non-polar organic chemicals (option)			
Fraction of organic carbon in aquifer	foc	1.00E-03	fraction
Organic carbon partition coefficient	Koc	5.25E+01	l/kg
Entry for ionic organic chemicals (option)			
Sorption coefficient for related species	$K_{oc,n}$		l/kg
Sorption coefficient for ionised species	$K_{oc,i}$		l/kg
pH value	pH		
acid dissociation constant	pKa		
Soil water partition coefficient	Kd	5.25E-02	l/kg

Dispersivity

Calculate dependant on distance to compliance point (0), specify dispersivity (1), or calc after Xu & Eckstein (2) ? **2**

		Enter value	Calc value	Xu & Eckstein	
Longitudinal dispersivity	**ax**	0.00E+00	5.00E+00	2.98E+00	m
Transverse dispersivity	**az**	0.00E+00	5.00E-01	2.98E-01	m
Vertical dispersivity	**ay**	0.00E+00	5.00E-02	2.98E-02	m

For calculated value, assumes ax = 0.1 *x, az = 0.01 * x, ay = 0.001 * x
Xu & Eckstein (1995) report $ax = 0.83(\log_{10}x)^{2.414}$; az = ax/10, ay = ax/100 are assumed



Note graph assumes plume disperses vertically in one direction only. An alternative solution assuming the centre of the plume is located at the mid-depth of the aquifer is presented in the calculation sheets.

This sheet calculates the Tier3 remedial target for groundwater, based on the distance to the receptor or compliance located down hydraulic gradient of the source Three solution methods are included, the preferred option is Ogata

By setting a long travel time it will give the steady state solution, which should be used to calculate remedial targets.

The measured groundwater concentration should be compared
with the Tier 3 remedial target to determine the need for further action.
Note if contaminant is not subject to first order degradation, then set half life as 9.0E+99.

Calculated concentrations for distance-concentration graph

Ogata Banks
From calculation sheet

Distance	**Concentration** **mg/l**
2.5	1.3E+00
5.0	1.2E+00
7.5	1.2E+00
10.0	1.1E+00
12.5	1.1E+00
15.0	1.0E+00
17.5	9.7E-01
20.0	9.3E-01
22.5	8.9E-01
25.0	8.5E-01
27.5	8.1E-01
30.0	7.8E-01
32.5	7.5E-01
35.0	7.1E-01
37.5	6.8E-01
40.0	6.5E-01
42.5	6.2E-01
45.0	6.0E-01
47.5	5.7E-01
50.0	5.5E-01

Site being assessed:	Fictional site
Completed by:	S Hohne
Date:	Enter date
Version:	x.xx

R&D Publication 20 Remedial Targets Worksheet, Release 2.2a

Tier 3 - Groundwater

Input Parameters (using pull down menu)

Input Parameters (using pull down menu)	Variable	Value	Unit	Source
Contaminant		**Benzene**		
Target Concentration	C_T	**3.00E-03**	mg/l	

Select analytical solution (click on brown cell below, then on pull-down menu)

Ogata Banks — **Equations in R&D Pub. 20**

Enter '1' to simulate vertical dispersion in one direction, '2' for two directions (pull down menu) **2**

Enter '1' if biodegradation rate is for the substance in water,
' if rate is for decay in field conditions (i.e. field data from aquifer) (pull down men **1**

	Variable	Value	Unit	Source of parameter value
Initial contaminant concentration in groundwater at plume core	C_0	1.60E-01	mg/l	*Measured*
Half life for degradation of contaminant in water	$t_{1/2}$	3.70E+02	days	*Howard, 1991*
Calculated decay rate	λ	1.87E-03	days^{-1}	
Width of plume in aquifer at source (perpendicular to flow)	Sz	1.00E+02	m	*Measured*
Plume thickness at source	Sy	1.00E+01	m	*Measured*
Saturated aquifer thickness	da	2.00E+01	m	*Measured*
Bulk density of aquifer materials	ρ	1.65E+00	g/cm^3	*Measured*
Effective porosity of aquifer	n	3.00E-02	fraction	*Measured*
Hydraulic gradient	i	4.00E-02	fraction	*Calculated*
Hydraulic conductivity of aquifer	K	3.00E-02	m/d	*Measured*
Distance to compliance point	x	5.00E+01	m	*Measured*
Distance (lateral) to compliance point perpendicular to flow direction	z	0.00E+00	m	*Given*
Distance (depth) to compliance point perpendicular to flow direction	y	0.00E+00	m	*Given*
Time since pollutant entered groundwater	t	9.90E+99	days	*time variant options only*
Parameters values determined from options				
Partition coefficient	Kd	8.78E-02	l/kg	*see options*
Longitudinal dispersivity	ax	2.984	m	*see options*
Transverse dispersivity	az	0.298	m	*see options*
Vertical dispersivity	ay	0.030	m	*see options*

Calculated Parameters

Calculated Parameters	Variable		
Groundwater flow velocity	v	4.00E-02	m/d
Retardation factor	Rf	5.83E+00	fraction
Decay rate used	λ	3.21E-04	d^{-1}
Rate of contaminant flow due to retardation	u	6.86E-03	m/d
Contaminant concentration at distance x, assuming one-way vertical dispersion	C_{ED}	1.99E-02	mg/l
Contaminant concentration at distance x, assuming two-way vertical dispersion	C_{ED}	1.99E-02	mg/l
Attenuation factor (one way vertical dispersion, C_O/C_{ED})	AF	8.03E+00	
Attenuation factor (two way vertical dispersion, C_O/C_{ED})	AF	8.06E+00	

Remedial Targets

Remedial Target	**LTC3**	**2.42E-02**	**mg/l**
Ogata Banks			

For comparison with measured groundwater concentration.

Distance to compliance point		**50**	**m**	
Concentration of contaminant at compliance point	**C_{ED}/C0**	**1.99E-02**	**mg/l**	Ogata Banks
after		**9.9E+99**	**days**	

Care should be used when calculating remedial targets using the time variant options as this may result in an overestimate of the remedial target.
The recommended value for time when calculating the remedial target is 9.9E+99.

Select Method for deriving Partition Co-efficient (using pull down menu)

Calculate for non-polar organic chemicals

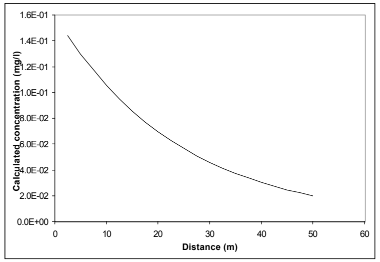
Entry if specify partition coefficient (option)			
Soil water partition coefficient	Kd		l/kg
Entry for non-polar organic chemicals (option)			
Fraction of organic carbon in aquifer	foc	1.00E-03	fraction
Organic carbon partition coefficient	Koc	8.78E+01	l/kg
Entry for ionic organic chemicals (option)			
Sorption coefficient for related species	$K_{oc,n}$		l/kg
Sorption coefficient for ionised species	$K_{oc,i}$		l/kg
pH value	pH		
acid dissociation constant	pKa		
Soil water partition coefficient	Kd	8.78E-02	l/kg

Dispersivity

Calculate dependant on distance to compliance point (0), specify dispersivity (1), or calc after Xu & Eckstein (2) ? **2**

		Enter value	Calc value	Xu & Eckstein	
Longitudinal dispersivity	**ax**	0.00E+00	5.00E+00	2.98E+00	m
Transverse dispersivity	**az**	0.00E+00	5.00E-01	2.98E-01	m
Vertical dispersivity	**ay**	0.00E+00	5.00E-02	2.98E-02	m

For calculated value, assumes ax = 0.1 *x, az = 0.01 * x, ay = 0.001 * x
Xu & Eckstein (1995) report $ax = 0.83(\log_{10}x)^{2.414}$; az = ax/10, ay = ax/100 are assumed



Note graph assumes plume disperses vertically in one direction only. An alternative solution assuming the centre of the plume is located at the mid-depth of the aquifer is presented in the calculation sheets.

This sheet calculates the Tier3 remedial target for groundwater, based on the distance to the receptor or compliance located down hydraulic gradient of the source Three solution methods are included, the preferred option is Ogata

By setting a long travel time it will give the steady state solution, which should be used to calculate remedial targets.

The measured groundwater concentration should be compared
with the Tier 3 remedial target to determine the need for further action.
Note if contaminant is not subject to first order degradation, then set half life as 9.0E+99.

Calculated concentrations for distance-concentration graph

Ogata Banks
From calculation sheet

Distance	**Concentration**
	mg/l
2.5	**1.4E-01**
5.0	**1.3E-01**
7.5	**1.2E-01**
10.0	**1.1E-01**
12.5	**9.5E-02**
15.0	**8.6E-02**
17.5	**7.7E-02**
20.0	**7.0E-02**
22.5	**6.3E-02**
25.0	**5.6E-02**
27.5	**5.1E-02**
30.0	**4.6E-02**
32.5	**4.1E-02**
35.0	**3.7E-02**
37.5	**3.4E-02**
40.0	**3.0E-02**
42.5	**2.7E-02**
45.0	**2.5E-02**
47.5	**2.2E-02**
50.0	**2.0E-02**

Site being assessed:	Fictional site
Completed by:	S Hohne
Date:	Enter date
Version:	x.xx

R&D Publication 20 Remedial Targets Worksheet, Release 2.2a

Tier 3 - Groundwater

ENVIRONMENT AGENCY

Input Parameters (using pull down menu)

Parameter	Variable	Value	Unit	Source
Contaminant		Anthracene		
Target Concentration	C_T	**5.00E-03**	mg/l	

Select analytical solution (click on brown cell below, then on pull-down menu)

Ogata Banks — **Equations in R&D Pub. 20**

Enter '1' to simulate vertical dispersion in one direction, '2' for two directions (pull down menu): **2**

Enter '1' if biodegradation rate is for the substance in water,
' if rate is for decay in field conditions (i.e. field data from aquifer) (pull down men: **1**

Parameter	Variable	Value	Unit	Source of parameter value
Initial contaminant concentration in groundwater at plume core	C_0	2.00E-02	mg/l	*Measured*
Half life for degradation of contaminant in water	$t_{1/2}$	5.10E+02	days	*Howard, 1991*
Calculated decay rate	λ	1.36E-03	$days^{-1}$	
Width of plume in aquifer at source (perpendicular to flow)	Sz	1.00E+02	m	*Measured*
Plume thickness at source	Sy	1.00E+01	m	*Measured*
Saturated aquifer thickness	da	2.00E+01	m	*Measured*
Bulk density of aquifer materials	ρ	1.65E+00	g/cm^3	*Measured*
Effective porosity of aquifer	n	3.00E-02	fraction	*Measured*
Hydraulic gradient	i	4.00E-02	fraction	*Calculated*
Hydraulic conductivity of aquifer	K	3.00E-02	m/d	*Measured*
Distance to compliance point	x	5.00E+01	m	*Measured*
Distance (lateral) to compliance point perpendicular to flow direction	z	0.00E+00	m	*Given*
Distance (depth) to compliance point perpendicular to flow direction	y	0.00E+00	m	*Given*
Time since pollutant entered groundwater	t	9.90E+99	days	*time variant options only*
Parameters values determined from options				
Partition coefficient	Kd	2.34E+01	l/kg	*see options*
Longitudinal dispersivity	ax	2.984	m	*see options*
Transverse dispersivity	az	0.298	m	*see options*
Vertical dispersivity	ay	0.030	m	*see options*

Calculated Parameters

Parameter	Variable	Value	Unit
Groundwater flow velocity	v	4.00E-02	m/d
Retardation factor	Rf	1.29E+03	fraction
Decay rate used	λ	1.06E-06	d^{-1}
Rate of contaminant flow due to retardation	u	3.11E-05	m/d
Contaminant concentration at distance x, assuming one-way vertical dispersion	C_{ED}	4.22E-03	mg/l
Contaminant concentration at distance x, assuming two-way vertical dispersion	C_{ED}	4.21E-03	mg/l
Attenuation factor (one way vertical dispersion, C_O/C_{ED})	AF	4.73E+00	
Attenuation factor (two way vertical dispersion, C_O/C_{ED})	AF	4.75E+00	

Remedial Targets

Remedial Target	**LTC3**	**2.38E-02**	**mg/l**

For comparison with measured groundwater concentration.

Ogata Banks

Distance to compliance point		**50**	**m**	
Concentration of contaminant at compliance point	**C_{ED}/C0**	**4.22E-03**	**mg/l**	Ogata Banks
after		**9.9E+99**	**days**	

Care should be used when calculating remedial targets using the time variant options as this may result in an overestimate of the remedial target.
The recommended value for time when calculating the remedial target is 9.9E+99.

Select Method for deriving Partition Co-efficient (using pull down menu)

Calculate for non-polar organic chemicals

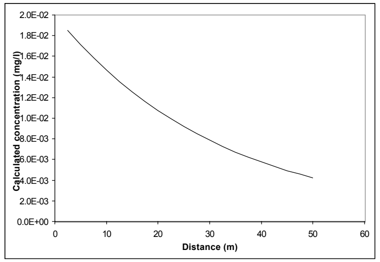
Parameter	Variable	Value	Unit
Entry if specify partition coefficient (option)			
Soil water partition coefficient	Kd		l/kg
Entry for non-polar organic chemicals (option)			
Fraction of organic carbon in aquifer	foc	1.00E-03	fraction
Organic carbon partition coefficient	Koc	2.34E+04	l/kg
Entry for ionic organic chemicals (option)			
Sorption coefficient for related species	$K_{oc,n}$		l/kg
Sorption coefficient for ionised species	$K_{oc,i}$		l/kg
pH value	pH		
acid dissociation constant	pKa		
Soil water partition coefficient	Kd	2.34E+01	l/kg

Dispersivity

Calculate dependant on distance to compliance point (0), specify dispersivity (1), or calc after Xu & Eckstein (2) ? **2**

		Enter value	Calc value	Xu & Eckstein	
Longitudinal dispersivity	**ax**	0.00E+00	5.00E+00	2.98E+00	m
Transverse dispersivity	**az**	0.00E+00	5.00E-01	2.98E-01	m
Vertical dispersivity	**ay**	0.00E+00	5.00E-02	2.98E-02	m

For calculated value, assumes ax = 0.1 *x, az = 0.01 * x, ay = 0.001 * x
Xu & Eckstein (1995) report ax = $0.83(\log_{10}x)^{2.414}$; az = ax/10, ay = ax/100 are assumed



Note graph assumes plume disperses vertically in one direction only. An alternative solution assuming the centre of the plume is located at the mid-depth of the aquifer is presented in the calculation sheets.

This sheet calculates the Tier3 remedial target for groundwater, based on the distance to the receptor or compliance located down hydraulic gradient of the source Three solution methods are included, the preferred option is Ogata

By setting a long travel time it will give the steady state solution, which should be used to calculate remedial targets.

The measured groundwater concentration should be compared
with the Tier 3 remedial target to determine the need for further action.
Note if contaminant is not subject to first order degradation, then set half life as 9.0E+99.

Calculated concentrations for distance-concentration graph

Ogata Banks
From calculation sheet

Distance	**Concentration**
	mg/l
2.5	**1.9E-02**
5.0	**1.7E-02**
7.5	**1.6E-02**
10.0	**1.5E-02**
12.5	**1.4E-02**
15.0	**1.3E-02**
17.5	**1.2E-02**
20.0	**1.1E-02**
22.5	**9.9E-03**
25.0	**9.2E-03**
27.5	**8.5E-03**
30.0	**7.9E-03**
32.5	**7.3E-03**
35.0	**6.7E-03**
37.5	**6.2E-03**
40.0	**5.8E-03**
42.5	**5.3E-03**
45.0	**4.9E-03**
47.5	**4.6E-03**
50.0	**4.2E-03**

Site being assessed:	Fictional site
Completed by:	S Hohne
Date:	Enter date
Version:	x.xx

R&D Publication 20 Remedial Targets Worksheet, Release 2.2a

Tier 3 - Groundwater

ENVIRONMENT AGENCY

Input Parameters (using pull down menu)

Input Parameters (using pull down menu)	Variable	Value	Unit	Source
Contaminant		Tetrachloethene		
Target Concentration	C_T	**5.00E-03**	mg/l	

Select analytical solution (click on brown cell below, then on pull-down menu)

Ogata Banks — **Equations in R&D Pub. 20**

Enter '1' to simulate vertical dispersion in one direction, '2' for two directions (pull down menu) **2**

Enter '1' if biodegradation rate is for the substance in water,
' if rate is for decay in field conditions (i.e. field data from aquifer) (pull down men **1**

	Variable	Value	Unit	Source of parameter value
Initial contaminant concentration in groundwater at plume core	C_0	7.35E-02	mg/l	*Measured*
Half life for degradation of contaminant in water	$t_{1/2}$	5.93E+02	days	*Howard, 1991; Thornton, 2000*
Calculated decay rate	λ	1.17E-03	$days^{-1}$	
Width of plume in aquifer at source (perpendicular to flow)	Sz	1.00E+02	m	*Measured*
Plume thickness at source	Sy	1.00E+01	m	*Measured*
Saturated aquifer thickness	da	2.00E+01	m	*Measured*
Bulk density of aquifer materials	ρ	1.65E+00	g/cm^3	*Measured*
Effective porosity of aquifer	n	3.00E-02	fraction	*Measured*
Hydraulic gradient	i	4.00E-02	fraction	*Calculated*
Hydraulic conductivity of aquifer	K	3.00E-02	m/d	*Measured*
Distance to compliance point	x	5.00E+01	m	*Measured*
Distance (lateral) to compliance point perpendicular to flow direction	z	0.00E+00	m	*Given*
Distance (depth) to compliance point perpendicular to flow direction	y	0.00E+00	m	*Given*
Time since pollutant entered groundwater	t	9.90E+99	days	*time variant options only*
Parameters values determined from options				
Partition coefficient	Kd	2.65E-01	l/kg	*see options*
Longitudinal dispersivity	ax	2.984	m	*see options*
Transverse dispersivity	az	0.298	m	*see options*
Vertical dispersivity	ay	0.030	m	*see options*

Calculated Parameters

Calculated Parameters	Variable		
Groundwater flow velocity	v	4.00E-02	m/d
Retardation factor	Rf	1.56E+01	fraction
Decay rate used	λ	7.50E-05	d^{-1}
Rate of contaminant flow due to retardation	u	2.57E-03	m/d
Contaminant concentration at distance x, assuming one-way vertical dispersion	C_{ED}	1.90E-02	mg/l
Contaminant concentration at distance x, assuming two-way vertical dispersion	C_{ED}	1.90E-02	mg/l
Attenuation factor (one way vertical dispersion, C_O/C_{ED})	AF	3.86E+00	
Attenuation factor (two way vertical dispersion, C_O/C_{ED})	AF	3.88E+00	

Remedial Targets

Remedial Target	**LTC3**	**1.94E-02**	**mg/l**	For comparison with measured groundwater concentration.
Ogata Banks				
Distance to compliance point		**50**	**m**	
Concentration of contaminant at compliance point	$C_{ED}/C0$	**1.90E-02**	**mg/l**	Ogata Banks
after		**9.9E+99**	**days**	

Care should be used when calculating remedial targets using the time variant options as this may result in an overestimate of the remedial target.
The recommended value for time when calculating the remedial target is 9.9E+99.

Select Method for deriving Partition Co-efficient (using pull down menu)

Calculate for non-polar organic chemicals

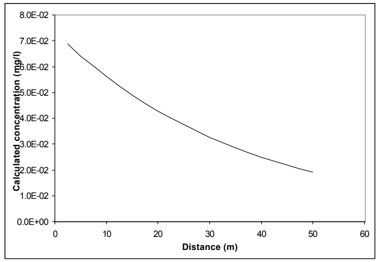
Entry if specify partition coefficient (option)			
Soil water partition coefficient	Kd		l/kg
Entry for non-polar organic chemicals (option)			
Fraction of organic carbon in aquifer	foc	1.00E-03	fraction
Organic carbon partition coefficient	Koc	2.65E+02	l/kg
Entry for ionic organic chemicals (option)			
Sorption coefficient for related species	$K_{oc,n}$		l/kg
Sorption coefficient for ionised species	$K_{oc,i}$		l/kg
pH value	pH		
acid dissociation constant	pKa		
Soil water partition coefficient	Kd	2.65E-01	l/kg

Dispersivity

Calculate dependant on distance to compliance point (0), specify dispersivity (1), or calc after Xu & Eckstein (2) ? **2**

		Enter value	Calc value	Xu & Eckstein	
Longitudinal dispersivity	**ax**	0.00E+00	5.00E+00	2.98E+00	m
Transverse dispersivity	**az**	0.00E+00	5.00E-01	2.98E-01	m
Vertical dispersivity	**ay**	0.00E+00	5.00E-02	2.98E-02	m

For calculated value, assumes ax = 0.1 *x, az = 0.01 * x, ay = 0.001 * x
Xu & Eckstein (1995) report ax = $0.83(\log_{10}x)^{2.414}$; az = ax/10, ay = ax/100 are assumed



Note graph assumes plume disperses vertically in one direction only. An alternative solution assuming the centre of the plume is located at the mid-depth of the aquifer is presented in the calculation sheets.

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By setting a long travel time it will give the steady state solution, which should be used to calculate remedial targets.

The measured groundwater concentration should be compared
with the Tier 3 remedial target to determine the need for further action.
Note if contaminant is not subject to first order degradation, then set half life as 9.0E+99.

Calculated concentrations for distance-concentration graph

Ogata Banks
From calculation sheet

Distance	Concentration mg/l
2.5	6.9E-02
5.0	6.4E-02
7.5	6.0E-02
10.0	5.6E-02
12.5	5.2E-02
15.0	4.9E-02
17.5	4.6E-02
20.0	4.3E-02
22.5	4.0E-02
25.0	3.7E-02
27.5	3.5E-02
30.0	3.3E-02
32.5	3.1E-02
35.0	2.9E-02
37.5	2.7E-02
40.0	2.5E-02
42.5	2.3E-02
45.0	2.2E-02
47.5	2.0E-02
50.0	1.9E-02

Site being assessed:	Fictional site
Completed by:	S Hohne
Date:	Enter date
Version:	x.xx