

Assessment of Aquifer Vulnerability in South Africa

Report to the
Water Research Commission

by

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Contents

<i>Acknowledgements</i>	<i>iii</i>
<i>Contents</i>	<i>iv</i>
<i>List of Tables</i>	<i>vii</i>
<i>List of Figures</i>	<i>ix</i>
<i>List of Appendices (enclosed on CD)</i>	<i>xi</i>
<i>Executive summary</i>	<i>xvi</i>

CHAPTER 1: INTRODUCTION 1

1.1 Background	1
1.2 Project objectives	2
1.3 Structuring the research	3
1.4 Report outline	4
1.5 References	4

CHAPTER 2: UNDERSTANDING AQUIFER VULNERABILITY 5

2.1 Unsaturated zone vulnerability	5
2.1.1 Factors controlling unsaturated zone vulnerability	6
2.2 Saturated zone vulnerability	8
2.2.1 Factors controlling the spatial extent of contamination	8
2.2.2 Factors controlling the persistence of contamination	9
2.3 References	11

CHAPTER 3: VULNERABILITY ASSESSMENT OF THE UNSATURATED ZONE 12

3.1 Existing approaches	12
3.2 The AQUISOIL vulnerability assessment approach	13
3.2.1 Sorption experiments	14
3.2.2 A new soil classification system for vulnerability assessment	17
3.3 The EUZIT vulnerability assessment approach	21
3.3.1 Thickness of the unsaturated zone	21
3.3.2 Hydraulic properties	22
3.3.3 Flow mechanism (preferential and matrix flow)	23
3.3.4 Travel time	24
3.3.5 Recharge	25
3.3.6 Slope	26
3.3.7 Sorption	26
3.3.8 Decay	27
3.3.9 Software application	28

3.4	References	31
CHAPTER 4: VULNERABILITY ASSESSMENT OF THE SATURATED ZONE		33
4.1	Two approaches for determining saturated zone vulnerability	33
4.2	Geochemical characteristics of primary and dual-porosity aquifers	34
4.2.1	Coastal primary aquifers	34
4.2.2	Dual-porosity, weathered zone aquifers	37
4.3	Saturated zone vulnerability - Geochemical and reactive transport models	40
4.3.1	Inorganic contaminant sources	40
4.3.2	Dissolved organic contaminant sources	44
4.4	Saturated zone vulnerability – Generic approach	46
4.4.1	Domenico mass transport equation	46
4.4.2	Saturated zone vulnerability indices	48
4.5	References	49
CHAPTER 5: GIS-BASED GROUNDWATER VULNERABILITY ASSESSMENT		51
5.1	AVAP's GIS-based approaches	51
5.2	Overview of UGIf Model	52
5.2.1	Assessment of recharge and pollutant fluxes in UGIf	53
5.2.2	Direct recharge	54
5.2.3	Non-Point Source (NPS) pollution flux model	56
5.3	Modified UGIf model	57
5.3.1	The Attenuation Factor(AF) model	58
5.3.2	Leaching Potential Index (LPI) model	59
5.3.3	Ranking Index(RI) model	59
5.3.4	Vulnerability of conservative contaminants	60
5.4	Data requirements and outputs	60
5.5	Software application	61
5.6	Limitations of UGIf and reliability of prediction	63
5.7	References	64
CHAPTER 6: CASE STUDIES		66
6.1	Goedehoop study site - Secunda	66
6.1.1	Conceptual model of the Goedehoop study site	67
6.1.2	Unsaturated zone vulnerability	68
6.1.3	Saturated zone vulnerability	74
6.1.4	Discussion	75
6.2	Coastal Park waste disposal site - Cape Town	76
6.2.1	Conceptual model of the Coastal Park waste disposal site	77
6.2.2	Unsaturated zone vulnerability	77
6.2.3	Saturated zone vulnerability	80
6.2.4	Discussion	81

6.3	Comparison of vulnerabilities at Coastal Park and Goedehoop	81
6.4	References	82
CHAPTER 7: A FRAMEWORK TO SUPPORT DECISION-MAKING		83
7.1	Groundwater vulnerability in a South African context	83
7.1.1	Water resource protection in South Africa	83
7.1.2	Water resource decision making	84
7.1.3	Uncertainty in vulnerability assessments	85
7.2	AVAP in a decision-making context	86
7.2.1	STAGE I: Screening and scoping	86
7.2.2	STAGE II: Vulnerability assessment	89
7.2.3	STAGE III: Decision-making	90
7.3	References	91

List of Tables

Table 3.1:	<i>Equations and regression coefficients for chemical envelopes relating to Cu and P sorption.....</i>	<i>16</i>
Table 3.2:	<i>Chemical vulnerability classes based on sorption behaviour and envelope equations.</i>	<i>18</i>
Table 3.3:	<i>Example of spreadsheet calculation of the chemical vulnerability classes to which a soil is assigned based on input values for six soil properties and employing the classification in Table 3.2.</i>	<i>19</i>
Table 3.4:	<i>Continuation of the example in Table 3.3 illustrating the incorporation of physical parameters into vulnerability classification and the way in which groundwater vulnerability is calculated when data for more than one layer or horizon is available.</i>	<i>20</i>
Table 3.5:	<i>Unsaturated zone thicknesses, type of media and resulting impact on groundwater vulnerability.....</i>	<i>22</i>
Table 3.6:	<i>Vertical hydraulic conductance and its impact on contaminant migration.</i>	<i>23</i>
Table 3.7:	<i>Percentage of smectitic clay fraction in the soil, depth to water table and resulting impact of groundwater vulnerability (low, medium or high).</i>	<i>24</i>
Table 3.8:	<i>Dominant flow mechanism in the unsaturated zone and resulting impact on groundwater vulnerability.....</i>	<i>24</i>
Table 3.9:	<i>Approximate flow velocities and vertical travel times (Maxe and Johansson, 1998). .</i>	<i>25</i>
Table 3.10:	<i>Unsaturated zone media type, travel time to water table and resulting impact on groundwater vulnerability for a 5 m thick unsaturated zone.</i>	<i>25</i>
Table 3.11:	<i>Unsaturated zone thickness, recharge and resulting impact on groundwater vulnerability.....</i>	<i>26</i>
Table 3.12:	<i>Slope, curvature and resulting impact on groundwater vulnerability.....</i>	<i>26</i>
Table 3.13:	<i>Contaminant persistence and sorption and its potential impact on groundwater.....</i>	<i>27</i>
Table 3.14:	<i>Unsaturated zone sorption capacity, contaminant persistence and resulting impact on groundwater vulnerability.</i>	<i>28</i>
Table 4.1:	<i>Comparison between seawater at high dilutions and rainwater collected at Cape Point.</i>	<i>34</i>
Table 4.2:	<i>Simulated compositions of recharge and groundwater in coastal primary aquifers. ..</i>	<i>37</i>
Table 4.3:	<i>Simulated composition of recharge water and groundwater in an inland, weathered zone.....</i>	<i>39</i>
Table 4.4:	<i>Composition of inorganic cocktails.....</i>	<i>40</i>
Table 4.5:	<i>Saturated zone vulnerability in coastal (primary) and weathered zone aquifers (after Campbell, 2005).</i>	<i>44</i>

<i>Table 6.1: Calculated vulnerability ratings for 12 soil profiles at Goedehoop in relation to profile location and soil classification.</i>	<i>70</i>
<i>Table 6.2: Vulnerability assessment of the Secunda site using unsaturated zone information (Jovanovic and Adams, 2007).</i>	<i>71</i>
<i>Table 6.3: Saturated zone vulnerability assessment results (after Campbell et al., 2005 and Usher et al., 2006).</i>	<i>75</i>
<i>Table 6.4: Vulnerability assessment of CFA using the Excel based unsaturated Zone Index Tool (Adams and Jovanovic, 2005; 2006).</i>	<i>78</i>
<i>Table 7.1: Overview of AVAPs' vulnerability assessment methods as applied to study areas.</i>	<i>90</i>

List of Figures

Figure 2.1: Schematic representation of unsaturated and saturated zones.	5
Figure 2.2: Processes influencing fate and behavior of waste constituents in the soil environment (modified from Burden and Sims, 1999).	6
Figure 2.3: Simplified conceptual framework of the attenuation capacity of an unsaturated zone.	7
Figure 2.4: Conceptual framework of the spatial dimension of saturated zone vulnerability (Appendix 7 ).	9
Figure 2.5: Conceptual framework of the factors influencing residence time of a contaminant in an aquifer (Appendix 7 ).	10
Figure 3.1: Cu sorption data for about 170 soils as a function of pH. The 0.95 and 0.05 quantile curves represent the chemical envelope of the Cu sorption data across the pH range.	15
Figure 3.2: Relationships between (a) Zn and Cu sorption and (b) sulfate and phosphate sorption in selected soils (n=60) calculated for a solution concentration of 1 mg L ⁻¹	17
Figure 3.3: Relationship between the various factors that determine the attenuation capacity of the unsaturated zone.	21
Figure 3.4: Screenshot of the main menu of the Excel-based Unsaturated Zone Index Tool (Appendix 26 ).	29
Figure 3.5: General scheme for determining the impact of the unsaturated zone on contaminant migration.	30
Figure 4.1: Components of the model of the chemical evolution of groundwater in a coastal aquifer.	36
Figure 4.2: Components of the model of chemical evolution of groundwater in a weathered zone.	39
Figure 4.3: Chloride concentration vs. time at the outflow point of the simulated aquifers, with continuous and single-pulse sources of contaminant mixtures.	41
Figure 4.4: Fluoride concentration against distance in the simulated coastal and weathered zone aquifers at time = 360 units (Appendix 7 ).	42
Figure 4.5: Lead concentration (moles/litre) and pH vs. time at specific distance from the source in coastal and weathered zone aquifers (Appendix 7 ).	43
Figure 5.1: Interface of the UGI _f model for assessing NPS BTEX pollutant fluxes.	53
Figure 5.2: Simplified flow chart for estimating pollutant mass fluxes at the water table.	54
Figure 5.3: The conceptual model for the direct recharge calculations.	55
Figure 6.1: The Goedehoop irrigation site with the Sasol Synfuels complex in the background	66
Figure 6.2: The Goedehoop irrigation site, showing streams and monitoring borehole locations.	67
Figure 6.3: Schematic cross-section through the Goedehoop study site.	68
Figure 6.4: Illustrative Chemical profiles for Cl, pH, B and F plotted for samples taken in 1991 and 2002 from a site at Indaba adjacent to Goedehoop (Ginster, 2004).	69
Figure 6.5: Profile vulnerability ratings for metal contaminants in relation to the S (=CEC) value.	70

Figure 6.6: Distribution of travel time in years for a conservative contaminant, with shorter travel times (darker colours) indicating higher vulnerability.	73
Figure 6.7: Leaching potential index values for Benzene in recharge water, where higher values (darker colours) indicate higher vulnerability.	74
Figure 6.8: The Coastal Park waste disposal site	76
Figure 6.9: The Coastal Park waste disposal site and monitoring boreholes.	76
Figure 6.10: Distribution of travel time in years for a conservative contaminant at Coastal Park, with shorter travel times (darker colours) indicating higher vulnerability.	79
Figure 6.11: Leaching index potential values for Benzene in recharge water at Coastal Park, where higher values (darker colours) indicate higher vulnerability.	80
Figure 7.1: Hierarchy of Environmental Assessment and Management Tools (DWAF 2002).	84
Figure 7.2: Schematic overview of aquifer vulnerability decision-making.	88

List of Appendices (enclosed on CD)

Appendix 1	Fey, 2004 , Motivation for selecting Secunda as a field study site/case history
	Minutes of 1 st project meeting
Appendix 2	Mongwe and Fey, 2004 , The buffering capacity of soil materials for various contaminant types and the relationship between soil morphology, chemical properties and buffering capacity
Appendix 3	Adams, Jovanovic, Thomas, Titus, Anthony, Majola, Jia, 2004 , Review of Groundwater Vulnerability Assessment Methods - Unsaturated Zone.
	Adams, Jovanovic, Thomas, Titus, Anthony, Majola, Jia, 2004 , Review of Groundwater Vulnerability Assessment Methods - Unsaturated Zone - Appendices.
Appendix 4	Campbell, 2004 , Contaminant buffering capacity of the saturated zone – a literature review.
Appendix 5	Herselman and Fey, 2004 , Selection of soil profiles for groundwater vulnerability assessment - laboratory sorption studies
	Excel spreadsheet of selected soils.
Appendix 6	Conrad, 2004 , Literature review of (i) GIS-based vulnerability assessment methods used to date, and (ii) related data uncertainty and error propagation.
Appendix 7	Campbell, 2005 , One-dimensional solute transport modelling of priority inorganic pollutants.
Appendix 8	Fey, Mongwe and Mwepu, 2005 , Attenuation of pollutants by a representative selection of South African soils.
Appendix 9	Adams and Jovanovic, 2005 , Testing and documenting suitable vulnerability assessment methods in key study area.
Appendix 10	Campbell, Botha and Beekman, 2005 , Reactive-transport modelling of irrigation effluent in the weathered zone aquifer at the Sasol Goedeheop site, Secunda.
Appendix 11	Collection, analysis, interpretation and documentation of field samples/data (soil, groundwater climatic and other data) from the key study areas (including compilation of data for a data retrieval system).
Appendix 12	Conrad and Thomas, 2005 , GIS-based algorithms for vulnerability assessment.
Appendix 13	Saayman and Beekman, 2006 , Aquifer vulnerability to pollution in urban catchments – a decision support system – Phase I.
Appendix 14	Thomas, Conrad and Munch, 2006 , Guidelines for developing and compiling groundwater vulnerability maps using GIS.
Appendix 15	Saayman and Beekman, 2007 , Aquifer vulnerability to pollution in urban

	catchments - A framework to support decision-making.
Appendix 16	Fey and Mwepu, 2006 , Assessment of pollutant attenuation – II (Deliverable 2.1) and Comprehensive guide to the diagnostic value of soil properties for prediction of attenuation by soils of different classes of pollutants (Deliverable 3.3)
Appendix 17	Adams and Jovanovic, 2006 , Refining suitable vulnerability assessment methods for local application including bimodal flow and the concept of pollutant travel time.
Appendix 18	Usher, Lenong and Pretorius, 2006 , Solute transport modelling of priority dissolved organic constituents.
Appendix 19	Fey, Mwepu and Steyn, 2007 , Contribution to the final report on groundwater vulnerability assessment.
	Fey, Mwepu and Steyn, 2007 , Case study: the impact of effluent irrigation at Secunda
	Excel spreadsheet: US-ISCW Secunda data
	Excel spreadsheet: US-ISCW Final analyses G3675 reworked Feb 9 2007.
	Excel spreadsheet: US-ISCW Aquifer vulnerability classification.
Appendix 20	Jovanovic and Adams, 2007 , Contribution to the final report on vulnerability assessment of the unsaturated zone (regolith) in different geohydrological environments.
Appendix 21	Beekman and Usher, 2007 , Contribution to final report on vulnerability assessment of the saturated zone
Appendix 22	AVAP short course announcement and course schedule
Appendix 23	Final GIS vulnerability maps
Appendix 24	AQUISOIL spreadsheet programme
	AQUISOL guide
Appendix 25	EUZIT spreadsheet programme
Data Files	GIS Files – DRASTIC Approach
	Soil Chemistry files - Secunda
	PhreeqC input and output files

Glossary

Aquifer: Permeable earth material such as porous sediments or fractured hard rock, saturated with groundwater. The permeability should be such that it is capable of conducting and yielding usable quantities of groundwater to a borehole(s) and / or springs (a supply rate of 0.1 L/s is considered as a useable quantity). Latin: aqua - water and ferre - to carry. (The National Water Act (1998) defines an aquifer as ‘a geological formation which has structures or textures that hold water or permit appreciable water movement through them’).

Aquitard: A confining bed that retards, but does not completely stop the flow of water to or from an adjacent aquifer. Although it does not readily release water to boreholes or springs, it may function as a storage chamber for groundwater.

Biodegradation: Biodegradation is the process by which organic substances are broken down by other living organisms. (source: www.wikipedia.org)

Chemical attenuation: The capacity of aquifer solids to remove dissolved or suspended contaminants from groundwater and retain them.

Clay: A detrital sedimentary particle with a size of less than 1/256 mm. Material which is plastic when wet and has no well-developed parting along the bedding plane, although it may display banding.

Confined aquifer: An aquifer which is overlain by a confining layer of low permeability. The groundwater is confined under pressure greater than atmospheric pressure such that if the aquifer is penetrated the water level may rise above the top of the aquifer.

Contamination: The introduction into the environment of any substance by the action of man.

Darcy's Law: Darcy's Law is used to calculate the rate at which groundwater is moving in porous media. It states that the rate of flow through a porous medium is proportional to the loss of head, and inversely proportional to the length of the flow path and is defined by the following equation:

$$Q = T i w$$

where:

Q = Discharge

T = Transmissivity

i = Groundwater gradient

w = Length of groundwater unit perpendicular to flow

Ecosystem: An interconnected and interacting system comprising living organisms - including animals, plants, fungi, and microorganisms - and their non-living environment.

Environmental Impact Assessment (EIA): An Environmental Impact Assessment (EIA) is an assessment of the likely influence a project may have on the environment. Environmental Impact Assessment can be defined as: The process of identifying, predicting, evaluating and mitigating the biophysical, social, and other relevant effects of development proposals prior to major decisions being taken and commitments made (IAIA, 1999). The purpose of the assessment is to ensure that decision-makers consider environmental impacts before deciding whether to proceed with new projects.

Environmental Management System (EMS): The Environmental Management System (EMS) is part of a management system of an organization (enterprise, authority, etc.), in which specific competencies, behaviours, procedures and demands for the implementation of an operational environmental policy of the organization are defined. (source: www.wikipedia.org)

Hydraulic conductivity: Describes the ease with which water can move through pore spaces or fractures. It depends on the intrinsic permeability of the material and on the degree of saturation. Saturated hydraulic conductivity, K_{sat} , describes water movement through saturated media. (source: www.wikipedia.org)

Leaching: Dissolution of substances in the soil and removal by percolating water.

Permeability: Refers to the ease with which a fluid can pass through a porous medium. In hydrogeology, permeability is often used synonymously with hydraulic conductivity, which specifically refers to the ease with which water is transmitted through a porous medium. It is defined as the volume of water discharged from a unit area of an aquifer under unit hydraulic gradient in unit time (expressed as $m^3/m^2/d$ or m/d).

Pollution: The National Water Act (Act No. 36 of 1998) defines pollution as the direct or indirect alteration of the physical, chemical or biological properties of a water resource so as to make it:

- a) less fit for any beneficial purpose for which it may reasonably be expected to be use;
- b) harmful or potentially harmful -
 - to the welfare, health of safety of human beings;
 - to any aquatic or non-aquatic organisms;
 - to the resource quality; or
 - to property

Preferential flow: The preferential movement of water through more permeable zones in the subsurface. (source: SAGWDT)

Primary aquifer: An aquifer in which water moves through the original interstices of the geological formation, e.g. pores between sand grains. This type of porosity is termed primary porosity.

Recharge: The addition of water to the saturated zone, either by the downward percolation of precipitation or surface water and/or the lateral migration of groundwater from adjacent aquifers. (source: SAGWDT)

Risk: The probability in a certain timeframe that an adverse outcome will occur in a person, a group of people, animals and/or the ecology of a specified area that is exposed to a particular dose or concentration of a hazardous agent. This is both a function of the level of toxicity of the hazardous agent and the level of exposure. (NEPC, 1999)

Risk Assessment: The process for estimating the potential impact of a chemical, biological or physical agent on humans, animals and the ecology. (NEPC, 1999)

Risk management: The human activity which integrates recognition of risk, risk assessment, developing strategies to manage it, and mitigation of risk using managerial resources. Ideally a prioritization process is followed whereby the risks with the greatest loss and the greatest probability of occurring are handled first, and risks with lower probability of occurrence and lower loss are handled in descending order. (source: www.wikipedia.org)

Sand: A detrital deposit in which the particle size range from 1/16 mm to 2 mm.

Saturated zone: That part of the geological stratum in which all the voids are filled with water under pressure greater than that of the atmosphere.

Secondary aquifer: An aquifer in which water moves through the secondary interstices, which are a result of post-depositional processes, such as joints and faults.

Sediment: Particles derived from rocks or biological material that have been transported by air or water.

Soil zone: The usually thin upper surface layer of the earth's crust comprising living organisms, organic matter, decomposed rock or unconsolidated sediments, water and gases with properties attributable to the interaction of its parent material, time, climate, fauna and flora. (source: SAGWDT)

Sorption: The attachment of an ion, molecule or compound to a charged surface of a particle, usually a clay or organic matter.

Strategic Environmental Assessments (SEAs): A system of incorporating environmental considerations into policies, plans and programmes. It is sometimes referred to as Strategic Environmental Impact Assessment. (source: www.wikipedia.org)

Unconfined aquifer: An aquifer whose upper surface (water table) is free to fluctuate.

Unsaturated zone: That part of the geological stratum above the saturated zone in which the voids contain both air and water.

Water table: The top of an unconfined aquifer, where the aquifer is fully saturated and the water pressure is equal to atmospheric pressure. Usually measured in metres below ground level or below top of casing.

References

IAIA, 1999, 'Principles of Environmental Impact Assessment Best Practice Practice', International Association For Impact Assessment, in cooperation with U.K. Institute of Environmental Assessment.

NEPC (National Environment Protection Council), 1999, National Environmental Protection (Assessment of Site Contamination) Measure, National Environmental Protection Council, December 1999.

SAGWDT (South African Groundwater Decision Tool), 2006 CD, Groundwater Dictionary.

Executive summary

This report presents the main findings of the WRC-funded four-year project on “Improved methods for vulnerability assessments and protocols for producing vulnerability maps, taking into account information on soils”, abbreviated as AVAP. The project fulfils one of the key recommendations of a strategy on groundwater protection research which was prepared by Sililo et al. (2001). For detailed information, the reader is referred to the enclosed CD which includes all deliverables of the project (Appendixes 1 to 25).

Aquifer vulnerability to contamination comprises two components: unsaturated zone vulnerability and saturated zone vulnerability. For the unsaturated zone, AVAP defined vulnerability as the ease with which groundwater (at the water table) may become contaminated by a contaminant source at the surface or in the unsaturated zone. For the saturated zone, vulnerability is defined as a function of the period of time after contaminating activities have ceased that a given contaminant can be detected in groundwater plus the volume of the aquifer throughout which the contaminant is above a preset concentration. The decision-maker could focus on either one of these vulnerabilities or in combination depending on the type of decision to be made. AVAP developed new approaches for assessing aquifer vulnerability.

Unsaturated zone vulnerability

For the unsaturated zone, the “AQUISOIL” (Aquifer Vulnerability Soil Assessment) approach and a modified DRASTIC approach, called “EUZIT” (Excel-based Unsaturated Index Tool) were developed. Both approaches can be used for assessing vulnerability at the water table.

AQUISOIL focuses on the soil zone as the “first line of defence” but can also be applied to the whole unsaturated zone down to the water table. AQUISOIL comprises three types of vulnerabilities which are rated for each single layer and weighted according to thickness; i.e. chemical, hydraulic and climatic vulnerability. With regards to chemical vulnerability, a new soil classification was developed which relates sorption to selected soil properties (pH, clay and organic carbon content, CBD extractable Fe and Al, and the sum of exchangeable cations for more than 170 soil samples representing major kinds of diagnostic horizons and materials in the South African soil classification), by means of so-called chemical envelope equations. These envelopes predict the upper limit of contaminant sorption to be expected at a specified value of each soil property and are based on the application of quantile regression (also referred to as stochastic frontier analysis) which provides a systematic method of determining ranges of a determinant variable over which sorption can be either potentially maximal or inevitably minimal. Chemical vulnerability classes have been defined accordingly for the retention of the following categories of contaminants: cationic (metals), anionic and non-polar organic. Hydraulic vulnerability is derived from a permeability index which is based on soil texture and the presence or absence of a cemented layer or horizon. The climatic vulnerability uses a leaching or recharge index calculated with one or other of the classical algorithms that take into account factors such as rainfall, surface runoff, profile storage, etc. AQUISOIL has been incorporated in a spreadsheet programme.

EUZIT is a spreadsheet-based modified DRASTIC (Aller et al., 1987) approach. The rating of the unsaturated zone is based on a combination of factors that contribute to the likelihood of contaminants reaching the saturated zone following the path of aquifer recharge. The factors considered are the unsaturated zone thickness, hydraulic properties (vertical hydraulic conductivity), flow mechanism (preferential and matrix), travel time, recharge (based on well established methods), slope, contaminant sorption and decay (degradation). Any of these factors can be disabled depending on site-specific conditions and the weightings for each factor are user defined. EUZIT also allows for a multi-layer unsaturated zone. The rating scores for each factor are combined in the main menu to yield the rating of the impact of vadose zone on aquifer or groundwater vulnerability. The EUZIT programme draws the rating for sorption from the chemical vulnerability part of the AQUISOIL spreadsheet programme. The vulnerability of an aquifer to contamination originating at the soil surface can be assessed using data that are readily available, that can be calculated or that can be estimated using the information provided in the database of EUZIT.

Saturated zone vulnerability

For the saturated zone, two approaches are proposed to determine its vulnerability to contamination: one approach that uses (numerical) geochemical and reactive transport models and a second, generic, approach that generalise contaminant transport by an analytical equation. AVAP concentrated on the first approach and evaluated for two common aquifer types in South Africa: coastal primary and dual porosity aquifers the aquifer vulnerability to inorganic contamination from landfill leachate, industrial effluent and acid mine drainage, assuming identical physical properties and contamination at the water table. PHREEQC-2 (Parkhurst and Appelo, 1999) was used for the calculations. Vulnerability of the saturated zone to contamination is expressed in terms of spatial impact and persistence of the contaminant. Realistic spatial and temporal scales are derived from the linking of PHREEQC-2 with a single or multi-species groundwater flow/transport model such as MT3DMS (Zheng and Wang, 1999). For the modelling of organic contamination, PHT3D (Prommer, 2003), BIOPLUME III and the LNAPL Guide (American Petroleum Institute, 2004) can be used for simulating reactive transport of BTEX (considered representative of petroleum hydrocarbons), and the BIOCHLOR code (Aziz et al., 2000) for chlorinated ethenes.

GIS-based vulnerability assessment

A Geographical Information System (GIS) enables the compilation of vulnerability maps combined with other infrastructural information so that the results can be easily related to by planners and decision makers. Two GIS approaches were developed to determine unsaturated zone vulnerability as part of the AVAP project: EUZIT incorporated in a GIS and the modified UGIf model.

EUZIT was integrated in a GIS to assess the variation in groundwater vulnerability across an area. By building the input datasets into a GIS and converting them to grids the EUZIT algorithms can be applied in GIS using the “map calculator” functions. Within the GIS it is also possible to carry out a sensitivity analysis to optimise the weightings (and ratings) per factor. Depending on the scale of the application and the degree of spatial variability, the possibility does exist, however, that the initial spatial variability is “lost” due to the relatively broad ranges within the rating classes. One could refine the rating classes to enhance spatial variability in vulnerability. Further work is thus recommended on refining the ratings based on the scale of the study and data availability and on scientifically motivating the weightings.

The UGIf model, which estimates recharge fluxes of organic pollutants (BTEX) in an urban environment (Thomas et al., 2001), was modified to include screening level models for vulnerability assessment such as the Attenuation Factor Model (Rao et al., 1985), the Leaching Potential Index Model (Meaks and Dean, 1990), the Ranking Index Model (Britt et al., 1992), and a simple approach to assessing intrinsic vulnerability of conservative contaminants. The three screening level algorithms of UGIf require a combined grid containing attributes of average recharge rate (m/day), soil moisture or volumetric water content, vadose zone depths (m), and the retardation factor values. The UGIf model was made suitable for South African conditions through the incorporation of representative land types. The software packages required to run UGIf model are ArcView GIS 3.x version (ver 3.1 or 3.2 or 3.3) and its extension Spatial Analyst.

Both EUZIT and UGIf deal exclusively with the vulnerability of the unsaturated zone. Both approaches are encouraged, as they present decision-makers with a spatial representation of unsaturated zone vulnerability.

Case studies

Two study sites were selected to illustrate the use of AVAP's approaches to the assessment of groundwater vulnerability: the Goedeheop irrigation site near Secunda, and the Coastal Park waste disposal site near Cape Town. It was found that the unsaturated zone vulnerabilities are relatively high for both aquifers. From the smaller travel times and higher leaching potential indices as derived from the AQUISOIL and EUZIT spreadsheet tools and the UGIf model it can be concluded that the unsaturated zone vulnerability to dissolved organic contaminants (e.g. BTEX) of the primary Cape Flats aquifer at Coastal Park is higher than the vulnerability of the dual porosity, weathered zone aquifer at the Goedeheop site. This means that contaminants generated at the surface are likely to reach the water table and pollute the aquifer sooner at the Coastal Park waste disposal site. The saturated zone vulnerability in terms of the spatial impact of inorganic and organic contamination is expected to be higher at the Coastal Park waste disposal site whereas the persistence is expected to be higher at the Goedeheop site. More detailed modelling, accounting for site specific physical properties, of the Cape Flats aquifer at the Coastal Park waste disposal site is needed to enable a better comparison of the saturated zone vulnerabilities of both aquifers.

Aquifer vulnerability and decision-making

Aquifer vulnerability assessments form an important input to managing the risk of water resource degradation. A framework to support decision-making was developed to assist groundwater vulnerability assessment practitioners in understanding the role of their assessments in groundwater management and to assist them in the selection of AVAP's approaches to groundwater vulnerability assessment. The framework highlights the fact that groundwater vulnerability assessments serve as input to contaminant risk assessments, which will in its part, contribute to a cost benefit analysis. It is the outcome of the cost benefit analysis which will ultimately inform decision-making. To guide the groundwater vulnerability assessor, a table is presented which briefly summarises AVAP's assessment approaches in terms of their limitations, applicability, accuracy, ease of use, and cost.

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CHAPTER 1:

INTRODUCTION

1.1 Background

The government of South Africa recognises the importance of protecting groundwater resources from pollution and hence the project “Protocols for assessing groundwater pollution impacts – formulation of a research strategy” was funded and implemented through the Water Research Commission (Sililo et al., 2001). The resulting strategy document provided a framework for further research in groundwater protection. One of the key recommendations of this strategy have been addressed in the WRC-funded project “Identification and prioritisation of groundwater contaminants and sources in South Africa’s urban catchments” (Usher et al., 2004). Other recommendations included the development of improved methods for vulnerability assessments and the development of methods for using available soils information in vulnerability assessments. These have been the focus of this WRC funded study on:

“Improved methods for aquifer vulnerability assessments and protocols for producing vulnerability maps, taking into account information on soils”

abbreviated as AVAP. The contaminant inventory project provided baseline data on the types of contaminants that pose a significant threat to groundwater, the environment and health in urban catchments and as such formed the basis for this project. The focus on urban catchments arises from the fact that the greatest variety and highest concentrations of pollution sources are found in these areas.

Aquifer vulnerability assessment is not a straightforward exercise as there is often a host of contributing physico-chemical factors. No single methodology can be suitably applied for all environments. Several methods of varying complexity have been developed and reported in the literature (e.g. Vrba and Zaporozec, 1994) but relatively few have been applied in South Africa (Sililo et al., 2001).

A major emphasis in the groundwater protection strategy (Sililo et al., 2001) was placed on further investigating the soil zone in developing and testing appropriate assessment methods. Existing techniques seldom consider soil properties in any level of detail and are generally based on soil thickness and physical properties such as grain size. Yet the soil is often the ‘first line of defence’ against the migration of contaminants to groundwater from overlying land-based activities, and soil chemical interactions can play a major role in the protection of aquifers. The determination of the attenuation capacity of the soil zone forms an important component of this study.

Whilst acknowledging the important role that the soil zone plays in pollutant attenuation, the research also focused on the unsaturated zone as a whole as well as on the saturated zone, thereby addressing the need to integrate soil and geologic information in vulnerability assessments, as called for in the strategy document and other publications (Sililo et al., 1999; 2001). Subsequent presentation of aquifer vulnerability in GIS-based maps is considered crucial in the proper planning, protection and management of groundwater resources. Vulnerability maps will provide information for groundwater resource classification and the implementation of source directed controls as required by the National Water Act (Act No. 36 of 1998).

1.2 Project objectives

The main objectives of the AVAP project are to:

1. Assess the pollutant attenuation capacity of soil horizons and other regolith materials and describe the diagnostic value of key morphological and chemical properties of soils for conveying information on their contaminant transport/attenuation potential;
2. Produce a special purpose classification of South African soils based on the binomial system, with attenuation capacity ratings as a basis for higher order groupings; special emphasis given to hillslope catenas and lateral movement in the landscape;
3. Incorporate hydrological inferences into the classification by identifying chemical affinities between groundwater and the overlying soil/regolith and their relationships to recharge characteristics;
4. Develop improved methods for vulnerability assessments in urban catchments; and
5. Produce guidelines for the development/compilation of vulnerability maps.

The first objective refers to the unsaturated zone as a whole with an emphasis on the soil zone. This objective, together with the 2nd and 3rd objectives formed the basis for objective 4: developing improved methods for vulnerability assessments in urban catchments. This project also developed improved methods for the saturated zone. Objective 5: the production of guidelines for the development/compilation of vulnerability maps was based on the outcomes of the previous objectives.

1.3 Structuring the research

In order to meet the challenges of this project, key scientists were selected from the following South African institutions: CSIR, IGS, US/ISCW, UWC and GEOSS representing the following research areas: Soil Chemistry (soil classification, trace metal mobility), Hydrogeology (unsaturated and saturated flow and solute transport), GIS (vulnerability mapping) and Decision Support. The vulnerability assessments focused on both ‘intrinsic’ and ‘specific’ vulnerability as defined in Vrba and Zaporozec (1994) with ‘intrinsic’ referring to hydrogeological factors only and ‘specific’ for both hydrogeological factors and an imposed contaminant load.

In order to meet the objectives of the project the following deliverables were produced by the researchers over a time span of four years (see enclosed CD ):

- Literature reviews on (i) the buffering capacity of soil materials for various contaminant types and the relationship between soil morphology, chemical properties and buffering capacity, (ii) vulnerability assessment tools (e.g. DRASTIC) for the unsaturated zone (regolith) and case studies in fractured rock dominated, urban, catchments, (iii) the buffering capacity of aquifer materials for various contaminant types, and (iv) GIS-based vulnerability assessment methods used to date and related data uncertainty and error propagation (Appendixes 2, 3, 4 and 6 );
- Unsaturated Zone: (i) assessment of pollutant attenuation by laboratory batch experiments on soil samples for selected organic and inorganic contaminants, (ii) developing a comprehensive guide to the diagnostic value of soil properties used in classification for prediction of attenuation by different classes of pollutants, and (iii) testing and documenting suitable vulnerability assessment methods for local application (two key study areas: Cape Flats and Secunda) including bimodal flow and the concept of pollutant travel time (Appendixes 5, 8, 9, 16 and 17 );
- Saturated Zone: (i) one-dimensional solute transport modelling of priority inorganic pollutants including various scenarios of pollutant migration to develop a generic framework for vulnerability assessment of the saturated zone, and (ii) construction of a flow and contaminant transport model for determining groundwater vulnerability of the Secunda-Goedehoop site for both inorganic and dissolved degradable organic contaminants (Appendixes 7, 10 and 18 );
- GIS-based vulnerability mapping and decision support: (i) development of GIS-based algorithms for producing maps, (ii) guidelines for the development and compilation of vulnerability maps and (iii) a framework to support decision-making (Appendixes 12, 13, 14 and 15 );
- Collection, analysis, interpretation and documentation of field samples/data (soil, groundwater climatic and other data) from the key study areas of Cape Flats and Secunda (Appendixes 1 and 11 ); and a
- Short course materials on groundwater vulnerability assessment and mapping with emphasis on the soil zone (Appendix 22 .

1.4 Report outline

This report is divided into 7 chapters:

- *Chapter 1*, this chapter, provides the background to the project, i.e. the context, objectives and structuring of the research;
- *Chapter 2* presents a generic framework for groundwater vulnerability assessment;
- *Chapters 3 and 4* discuss AVAP's methods for vulnerability assessment in the unsaturated (including the soil zone) and saturated zones;
- *Chapter 5* focuses on AVAP's GIS-based vulnerability assessments;
- *Chapter 6* illustrates the application of AVAPs' methods for two case studies: i.e. Goedeheop irrigation site near Secunda and the Coastal Park Waste Disposal Site;
- *Chapter 7* places the outcome of the AVAP project in a decision-making context.

1.5 References

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CHAPTER 2:

UNDERSTANDING AQUIFER VULNERABILITY

Both physical and chemical processes within the unsaturated and saturated zones control the impact of contamination. Specifically, the residence time of a contaminant in soil moisture or groundwater, and the distance that it travels are considered important measures of vulnerability. The AVAP project has focused on assessing vulnerability at a site specific scale in urban catchments. Aquifer vulnerability to contamination comprises two components: unsaturated zone vulnerability and saturated zone vulnerability.

2.1 Unsaturated zone vulnerability

Unsaturated zone vulnerability is defined as the ease with which groundwater (at the water table) may become contaminated by a contaminant source at the surface or in the unsaturated zone (Figure 2.1). It is controlled by the nature of the strata overlying the saturated zone and the nature of the contaminant or contaminant mixture (see Appendixes 3, 4 and 9 .

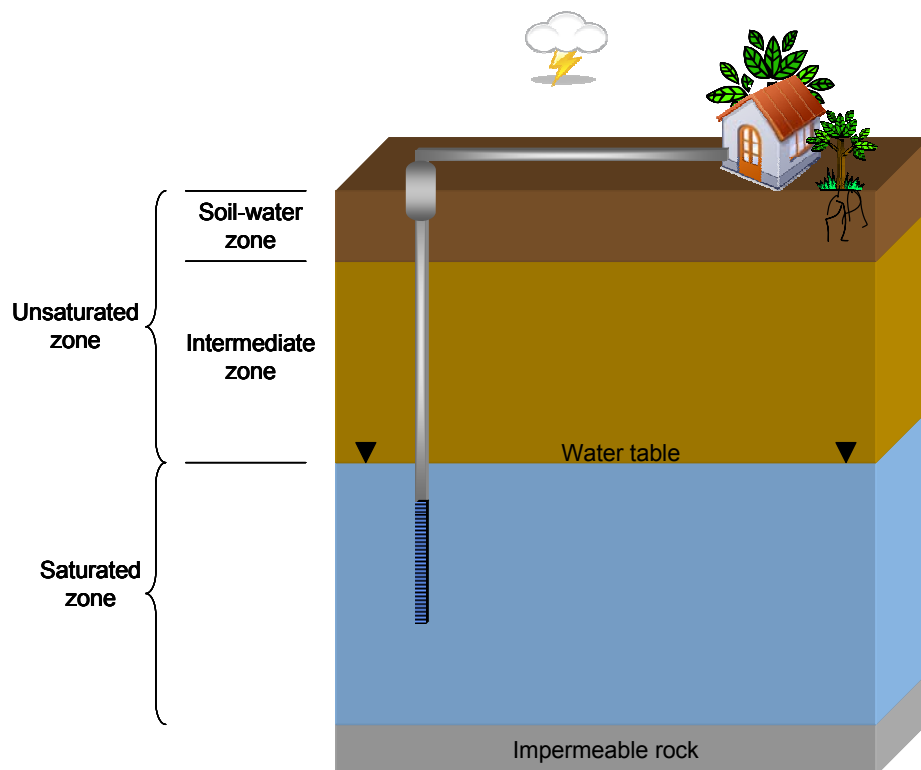


Figure 2.1: Schematic representation of unsaturated and saturated zones.

2.1.1 Factors controlling unsaturated zone vulnerability

Several factors can alter the concentration of pollutants in the soil and intermediate zone as shown in Figure 2.2, including (after NRC, 1993):

- The composition of the unsaturated zone, which can greatly influence transformations and reactions. For example, high organic matter or clay content increases sorption and thus lessens the potential for contamination.
- The depth to the water table, is an important factor as short flow paths decrease the opportunity for sorption and biodegradation, thus increasing the potential for contaminants to reach groundwater. Conversely, longer flow paths from land surface to the water table lessen the potential for contamination from chemicals that adsorb or degrade along the flow path. Preferential flow pathways in the unsaturated zone however, potentially allow contaminants to pass into the saturated zone relatively quickly.
- Groundwater recharge rates, which affect the extent and rate of transport of contaminants through the unsaturated zone.
- Finally, environmental factors, such as temperature, pH and water content, can significantly influence the degradation of contaminants by microbial transformations.

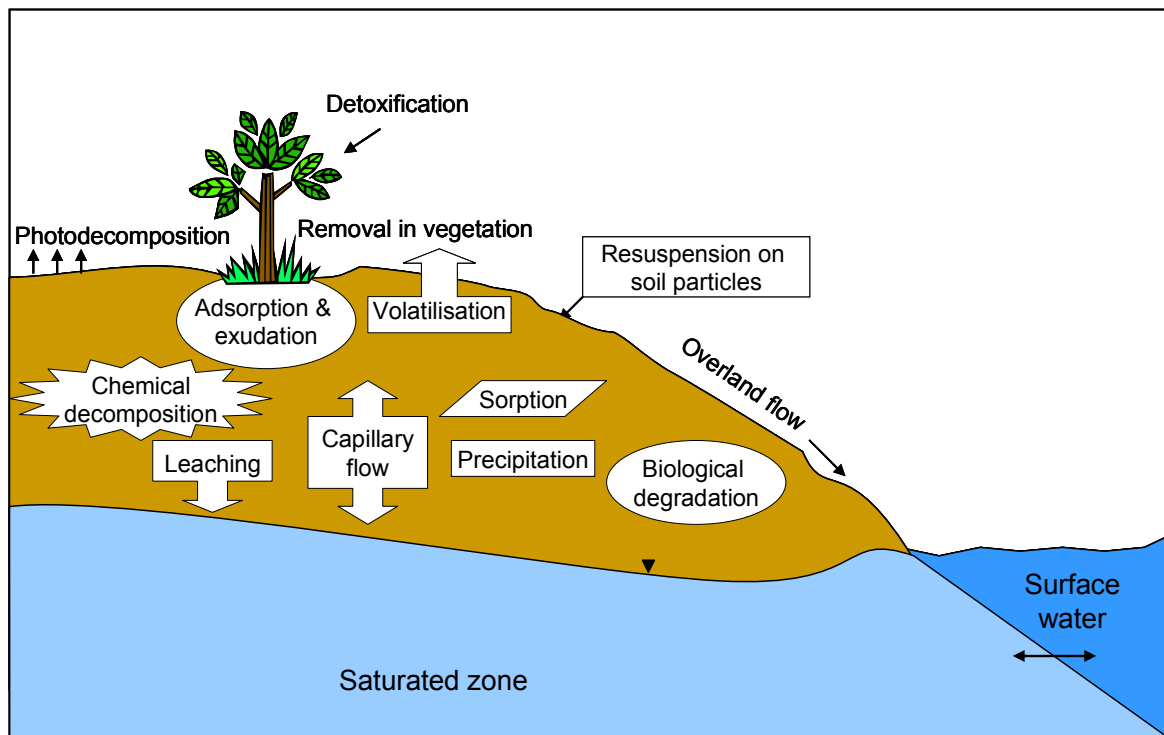


Figure 2.2: Processes influencing fate and behavior of waste constituents in the soil environment (modified from Burden and Sims, 1999).

Scanlon et al. (1997) indicated some important attributes that need to be considered when dealing with contaminant transport in the unsaturated zone: i.e. direction and rate of water movement; spatial and temporal variability of water fluxes; the type of medium (porous or fractured) because of the higher potential for preferential flow in fractured systems; the presence of vegetative cover as it removes much of the water from the surface; and the surface topography as it controls the movement of water by concentrating unsaturated flow in topographic depressions. These factors are in most cases interdependent and assume relative importance from site to site.

Unsaturated zone vulnerability is largely determined by the interplay between preferential and inter-granular flow, which controls the relative importance of chemical attenuation processes. The more preferential flow dominates, the less important chemical attenuation becomes, and vice versa. This is because preferential flow is relatively rapid and results in a relatively small surface area of contact between the infiltrating water and the solid matrix, compared with diffuse, inter-granular flow. Preferential flow makes transport difficult to predict and measure in the unsaturated zone. Micro- and macro-pore exchange fluxes, as well as preferential flow are therefore complicating factors in estimating travel times of contaminants through the unsaturated zone. A simplified conceptual framework of the attenuation capacity of the unsaturated zone (including the soil zone) that considers hydraulic and chemical attenuation is given below:

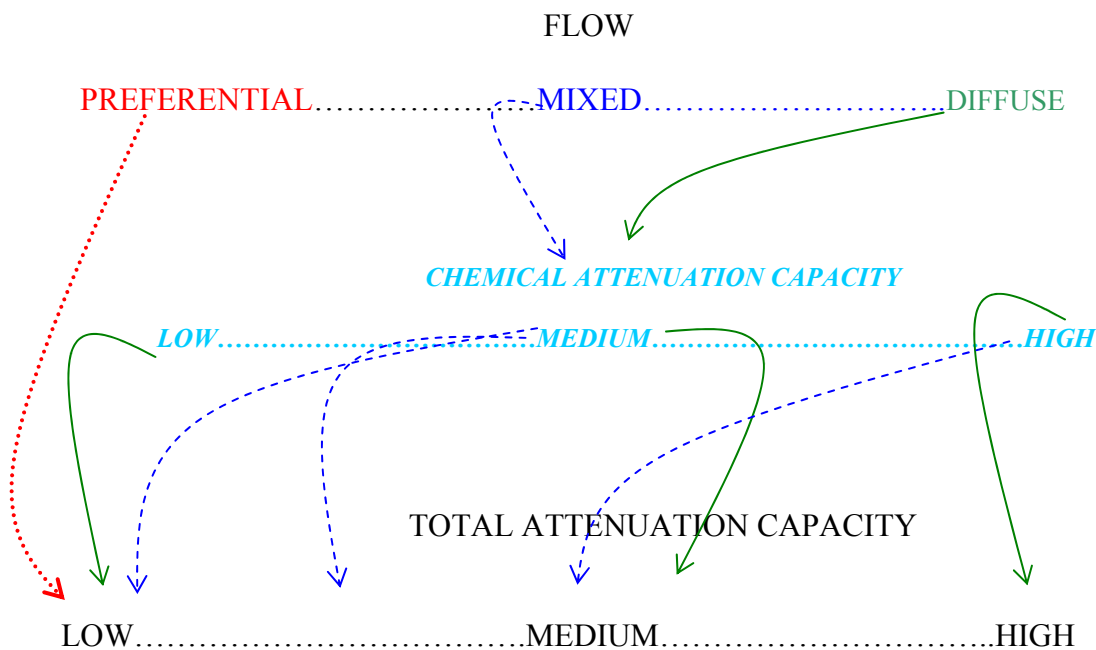


Figure 2.3: Simplified conceptual framework of the attenuation capacity of an unsaturated zone.

Lower attenuation means higher vulnerability of the underlying groundwater. More recharge for a given mass of contaminant – i.e. a finite source – implies that the concentration of contaminant moving through the unsaturated zone will be more dilute, thus the impact on

aquifer water quality less severe. However, the more recharge there is in a given period, the more rapidly a given mass of contaminant – dissolved or as mobile colloidal matter - will be transported through the unsaturated zone. The two processes usually do not impact on vulnerability in the same magnitude. In addition, the intensity and duration of rainfall events will determine the nature and magnitude of recharge.

In its simplest form the principal geologic and hydrogeologic features that will influence an aquifer's vulnerability from the unsaturated zone perspective are:

- Low Vulnerability – Thick unsaturated zone, with high levels of clay and organic material; and
- High vulnerability – Thin unsaturated zone, with high levels of sand, gravel or fractured rocks with high permeability.

2.2 Saturated zone vulnerability

Saturated zone vulnerability to contamination is considered a function of the period of time after contaminating activities have ceased that a given contaminant can be detected in groundwater and the volume of the aquifer throughout which the contaminant is above a preset concentration.

2.2.1 Factors controlling the spatial extent of contamination

The same factors apply to the saturated zone as to the unsaturated zone, i.e. the greater the dominance of in-fracture flow as opposed to diffuse/matrix (primary) flow, the less influence chemical attenuation has. The flow velocity also has an influence – the faster groundwater moves the further contaminated groundwater will move from its source in a given time period. The spatial distribution of the contaminant will also be controlled by the nature of flow in the aquifer. Fracture-controlled flow will, by definition, constrain the contaminant's spread within the fracture network. Matrix flow will be constrained by spatial variations in hydraulic conductivity. Chemical diffusion is important at much lower flow rates. A conceptual framework of the factors controlling the spatial distribution of a contaminant in the saturated zone (aquifer) is depicted in Figure 2.4. The scales are relative and approximate, and the diagram indicates the relative effects of the contributing factors over a fixed period of time.

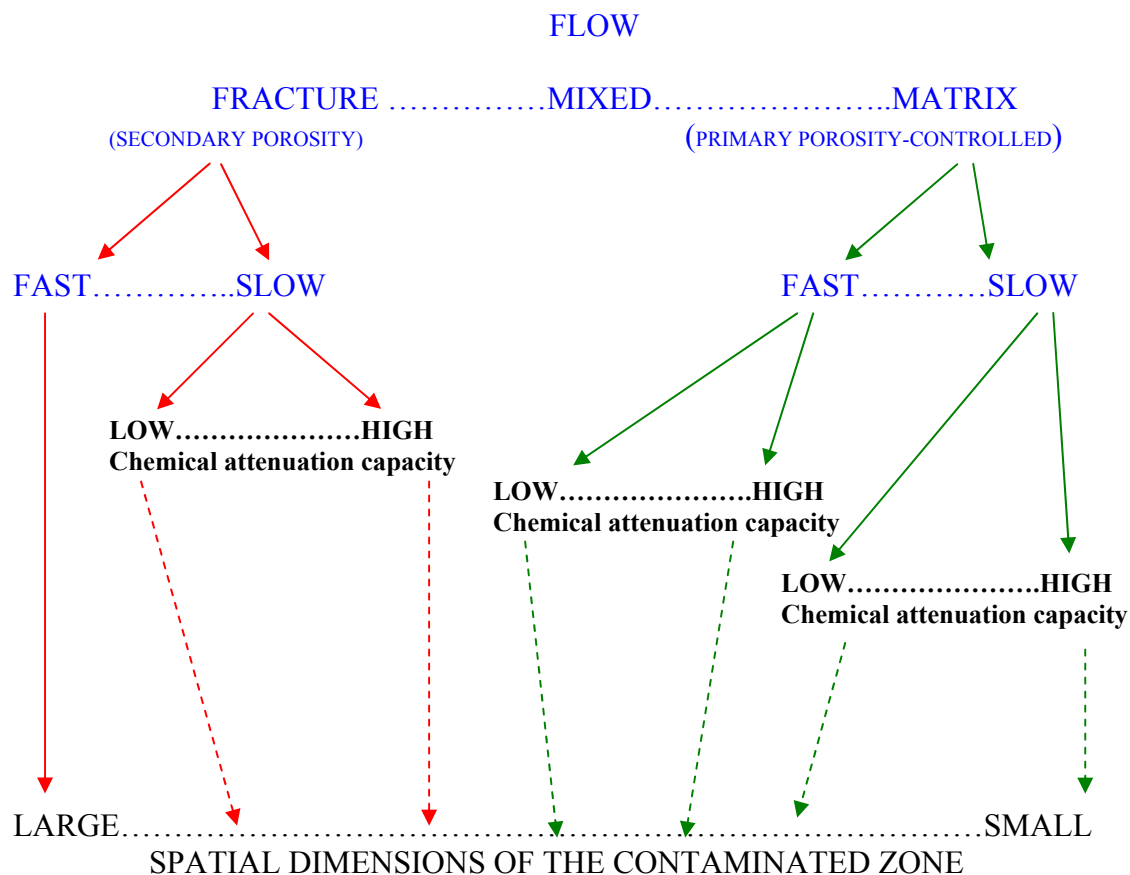


Figure 2.4: Conceptual framework of the spatial dimension of saturated zone vulnerability (Appendix 7 )

2.2.2 Factors controlling the persistence of contamination

Dilution

The concentration of a contaminant is largely controlled by the rate at which dilution of a contaminant plume takes place in the aquifer. The main factor influencing dilution is the magnitude of recharge relative to the volume of the contaminated zone and recharge results in a change in the shape and extent of the contaminated zone. Faster flow velocities will also cause more dilution through dispersive processes. Conversely, low velocities result in less dispersion and, in extreme cases in fractured aquifers, contaminants may become trapped in the “dead-ends” of fracture networks with low interconnectivity. Dilution would then be driven by chemical diffusion, and takes place very slowly.

Chemical attenuation

Chemical attenuation is the capacity of aquifer solids to remove dissolved or suspended contaminants from groundwater and retain them. An increase in residence time is controlled by dissolution and de-sorption rates of contaminants adsorbed to the solid phase. A

conceptual framework of the factors which influence the residence time of a contaminant in the saturated zone is shown in the figure below.

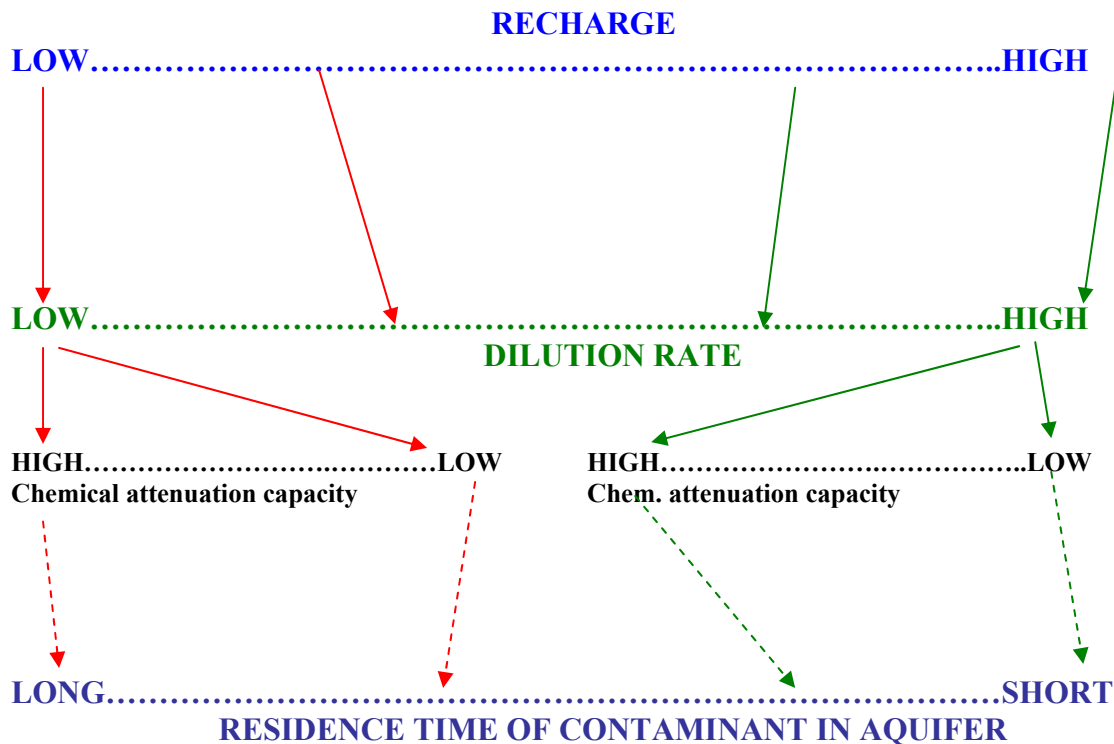


Figure 2.5: Conceptual framework of the factors influencing residence time of a contaminant in an aquifer (Appendix 7 .

Decay or decomposition

Most organic compounds and other chemical species, such as for example the nitrate ion, are consumed by reactions which reduce their concentration in aquifers. It is possible to assess the rate of these reactions, and include this factor in a determination of residence time. Radioactive isotopes have limited life spans as a result of radioactive decay. The decay rate has a well-defined value which allows the maximum residence time of the isotope in an aquifer to be calculated.

Volatilisation and multi-phase partitioning

Some contaminants may be either volatile, insoluble or partially soluble in water (multi-phase partitioning), including a non-aqueous phase liquid (NAPL) form. Partitioning coefficients are used to describe the partitioning of a chemical into these different phases. The fluxes of NAPL chemicals in liquid and non-liquid phase can be estimated from the relative permeability and proportion of air, water and NAPL saturation in porous media.

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CHAPTER 3:

VULNERABILITY ASSESSMENT OF THE UNSATURATED ZONE

The intrinsic geohydrological characteristics of the layer or layers above an aquifer and the physio-chemical properties of specific contaminants will determine the vulnerability of groundwater to pollution. As such, the unsaturated zone, especially the soil zone, represents the “first line of defence”. The unsaturated zone provides protection through (Harter and Walker, 2001):

- Intercepting, sorbing and eliminating pathogenic viruses and bacteria;
- Sorbing and degrading many synthetic organic chemicals; and
- Attenuating heavy metals and organic chemicals through sorption and complexation with mineral surfaces within the unsaturated zone and through uptake into plants and crops.

This chapter presents improved methods for assessing the vulnerability of groundwater to contamination based on the properties of the unsaturated zone.

3.1 Existing approaches

Several approaches or methods have been developed for assessing groundwater vulnerability. They range from sophisticated models of the physical, chemical and biological processes occurring in the unsaturated zone and groundwater regime, to models that weigh critical factors affecting vulnerability through either statistical methods or expert judgment. According to Van der Heijde (1996), the International Ground Water Modelling Center is informed every week of new computer codes addressing some aspects of fluid flow and contaminant behaviour in the subsurface. The number of inputs required generally depends on the level of complexity of the model. The National Research Council (NRC, 2001) identified the importance of conceptualizing (1) the relevant process, (2) the structure of the subsurface, and (3) the potential events or scenarios that impact the behaviour of the modeled system in unsaturated zone transport models. Conceptual models for partially saturated flow and transport in the fractured unsaturated zone environments are generally poorly developed and untested (NRC, 2001). There are a large number of modelling codes that can simulate surface water flow, subsurface water flow and contaminant fate and transport. However, each of these codes is based on different assumptions chosen for the purpose of simulating specific scenarios. No single code can be used to simulate all possible situations. In general, the intermediate zone (above the water table and below the soil zone) is also less researched than the soil and saturated zones.

Existing vulnerability assessment techniques, however, seldom consider soil properties in any level of detail. Yet the soil is often the ‘first line of defence’ against the migration of contaminants to groundwater from overlying land-based activities, and soil chemical interactions can play a major role in the protection of aquifers. A new classification methodology was therefore developed for South African soils to assess the contribution of the soil zone to unsaturated zone vulnerability (see Section 3.2).

The National Research Council (1993) classified (unsaturated zone) vulnerability assessment methods into three major classes: (1) overlay and index methods that combine specific physical characteristics that affect vulnerability, often giving a numerical score, (2) process-based methods consisting of mathematical models that approximate the behaviour of substances in the subsurface environment, and (3) statistical methods that draw associations with areas where contamination is known to have occurred.

One of the most popular overlay and index method used in South Africa is DRASTIC (Aller et al., 1987). This method has been, however, criticized in the past due to its subjectivity, its failure to consider some important geohydrological characteristics (including soil structure and preferential flow) and specific contaminant properties.

The design of an improved approach to groundwater vulnerability assessment needs to incorporate the following elements:

- a) Inclusion of multi-layer components for regolith material.
- b) Determination of hydraulic properties in the unsaturated zone (e.g. hydraulic conductivity, porosity and water retention).
- c) Inclusion of preferential flow, in particular short-circuiting (e.g. through soil cracks and fractures) and funneling (e.g. lateral transport of water and contaminants).
- d) Inclusion of chemical properties (e.g. solubility, volatilization, sorption and degradation) of specific contaminants and mixtures of contaminants.

For the purpose of improving groundwater vulnerability assessment, the project developed two new approaches: the “AQUISOIL” approach (Aquifer Vulnerability Soil Assessment; Section 3.2) focusing on the soil zone and a modified DRASTIC approach “EUZIT” (Excel-based Unsaturated Zone Index Tool; Section 3.3). Either approach can be used for assessing groundwater vulnerability at the water table.

3.2 The AQUISOIL vulnerability assessment approach

A new classification system was developed for South African soils for determining contaminant attenuation, based on properties inferred from the definitions of diagnostic horizons and materials in the current general purpose SA classification system (Soil Classification Working Group, 1991). When combined with physical parameters (hydraulic and climatic) the contribution of regolith to groundwater vulnerability can be determined.

3.2.1 Sorption experiments

Soil properties to which sorption behaviour is commonly related, namely: pH, the content of clay, organic carbon, and citrate-bicarbonate-dithionite (CBD)-extractable Fe and Al, and S value (the sum of exchangeable basic cations) were determined for more than 170 soil samples representing major kinds of diagnostic horizons and materials in the South African soil classification. For the purpose of grouping soils according to their chemical attenuation capacity, three classes of contaminants were considered (Sililo et al. 2001): (i) cationic; (ii) anionic; and (iii) non-polar organic substances. The sorption experiments carried out during the course of this project focused on the first two categories of contaminants since the adsorption of these is influenced by a variety of soil properties and is not amenable to simple prediction based on a single property, as is the case with the third category of contaminant.

In order to test whether the current South Africa soil classification (Soil Classification Working Group, 1991) is capable of predicting sorption behaviour, the mean and standard deviation of Cu or P sorption using CuCl_2 , and KH_2PO_4 at 1 mg/L solution concentration and a background concentration of 0.01 M CaCl_2 , for each of the major diagnostic horizons were calculated (see Appendix 19 for further details ). An equilibrium concentration of 1 mg/L was selected partly for convenience (since this corresponds directly with the intercept value on a logarithmic plot of the sorption isotherm equation) and partly in the realization that for many ionic contaminants a higher concentration than this would significantly exceed the environmentally meaningful lower limit whereas a lower concentration might, depending on the analytical method employed, entail undesirable error. The sorption data for different soil horizons revealed that the current classification fails to enable prediction of sorption characteristics, at least at the level of the soil form.

Accordingly, sorption capacities for Cu and P were compared with the selected soil properties of pH, clay content, organic carbon, and CBD-extractable Fe and Al, and S value. The analysis showed that there is no significant correlation between sorption capacity and any of the soil properties selected (see e.g. the scatter plot for Cu versus pH - Figure 3.1a). In many cases, however, it is possible to identify a range, of the determinant variable, over which the sorption capacity is predictably minimal and another range over which it is potentially maximal. The method of segmented quantile regression analysis was applied to the data to delineate the boundary to plots of observed measurements (Mills et al., 2006). Graphs showing a chemical envelope for either Cu or P represent a transformation of the corresponding scatter plots, in which the data have been segmented into 10 groups of equal sample size ($n=17$) based on the determinant variable, following which the 0.95 and 0.05 quantiles of the sorption values were calculated for each group (see Figure 3.1b as an example). Equations were fitted to the plotted values of the 0.95 quantile for each segment and these are presented along with their r^2 values in Table 3.1, which shows that in the case of Cu sorption, only three of the determinant variables (clay content, S value and pH) showed chemical envelopes on the basis of which an upper limit to sorption could reliably be

predicted whereas in the case of P, each one of the six selected soil properties proved to be reliable as a basis for predicting the upper limit to sorption.

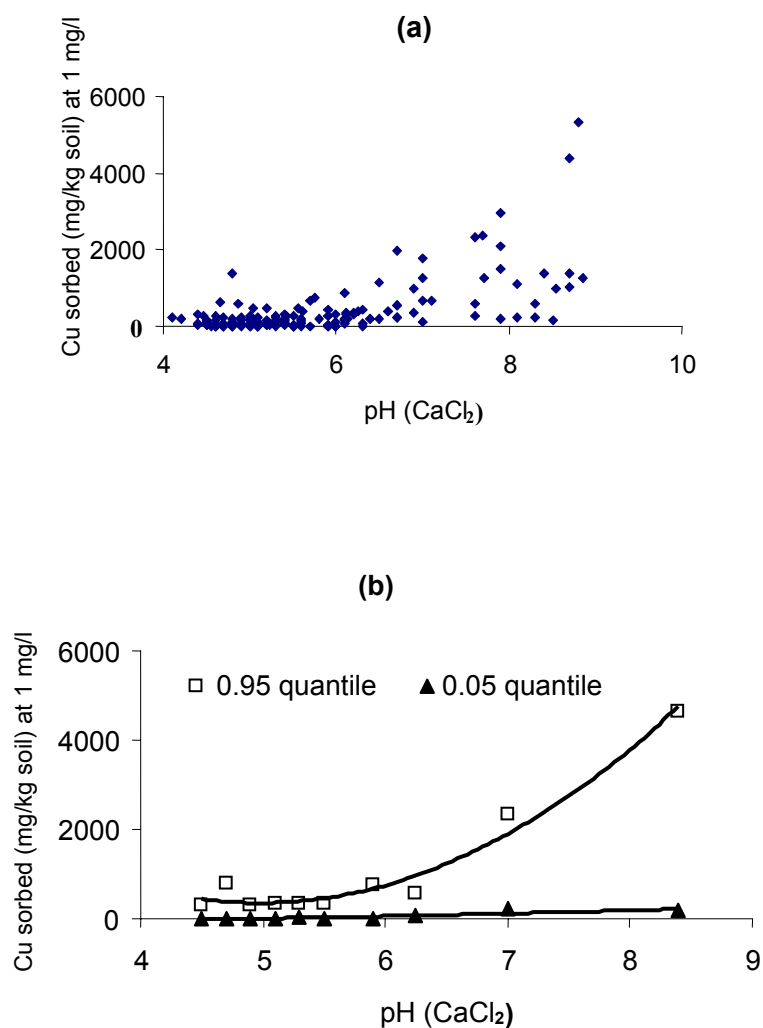


Figure 3.1: Cu sorption data for about 170 soils as a function of pH. The 0.95 and 0.05 quantile curves represent the chemical envelope of the Cu sorption data across the pH range.

Table 3.1: Equations and regression coefficients for chemical envelopes relating to Cu and P sorption.

Variable	Equation*	r ²
Copper		
S value (cmol _c kg ⁻¹)	y = 132x + 82	0.97
pH (CaCl ₂)	y = 393x ² - 3563x + 8426	0.97
C (%)	y = -243x ² + 601x + 509	0.05
Al (%)	y = 1072x ² - 2676x + 2074	0.25
Fe (%)	y = 1110x ^{0.1867}	0.11
Clay (%)	y = 663e ^{0.025x}	0.59
Phosphate		
S value (cmol _c kg ⁻¹)	y = 1279e ^{-0.043x}	0.80
pH (CaCl ₂)	y = 5222e ^{-0.33x}	0.69
C (%)	y = -35x ³ - 97x ² + 1088x + 299	0.82
Al (%)	y = 1220x + 333	0.95
Fe (%)	y = 198x + 267	0.91
Clay (%)	y = 76x ^{0.71}	0.77

* y = 0.95 quantile of sorption in mg kg⁻¹ at a solution concentration of 1 mg L⁻¹ corresponding to the determinant variable x.

The chemical envelopes can be used for the analysis of soil chemical processes. For instance, the quadratic behaviour of P sorption in relation to C content suggests that the association of increased soil C levels with higher rainfall and therefore a more weathered, acidic condition conducive to P retention is offset, in the higher part of the C range, by the smothering effect which humic substances are known to have on P sorbing surfaces.

A small selection of soils was used to test the sorption of Zn (using ZnCl₂) and sulfate (using KHSO₄) for comparison with Cu and phosphate sorption, respectively, to determine the feasibility of using observed Cu and P sorption behaviour as a means for anticipating cation and anion sorption in general (see Figure 3.2). Although the relationships are not strong, some correlation is evident, which implies that the assumption of Cu and P being representative of cations and anions is not seriously misplaced, especially if the objective is to create a small number of broad classes in terms of contaminant attenuation..

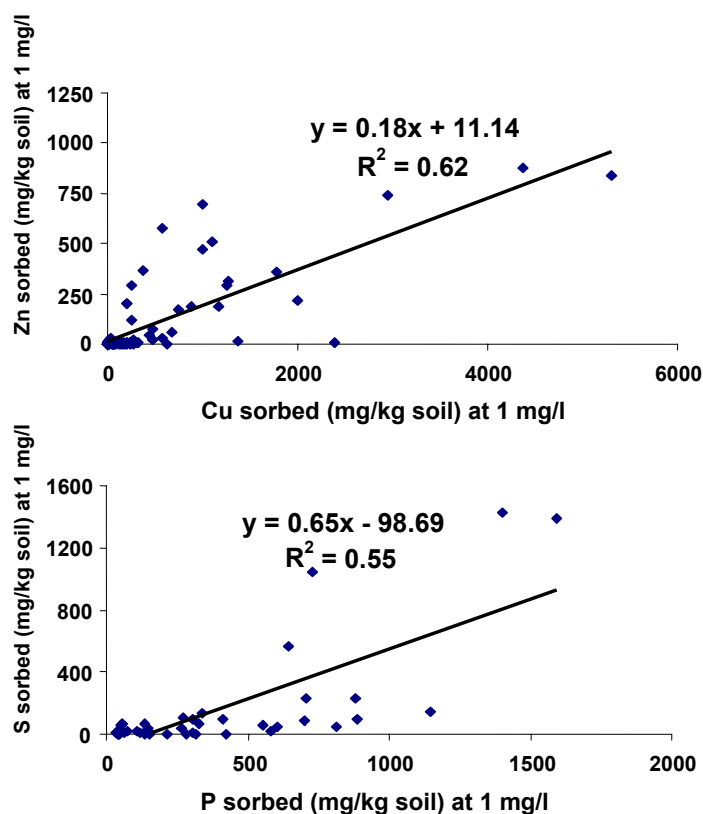


Figure 3.2: Relationships between (a) Zn and Cu sorption and (b) sulfate and phosphate sorption in selected soils (n=60) calculated for a solution concentration of 1 mg L⁻¹.

3.2.2 A new soil classification system for vulnerability assessment

Based on the chemical envelopes, the ranges of those soil properties to which sorption potential appears to be significantly related (pH, S value and clay content in the case of cations and each of the six properties in the case of anions) can be divided into three vulnerability classes (high, moderate, low) on the basis of their correspondence to ranges of sorption potential (see Table 3.2). Ranges for three soil properties are proposed for metals, six properties for anions or polar organics, and one (carbon content) for non-polar organics (based on the widely used K_{OC} concept which recognizes that sorption of non-polar organic molecules is regulated primarily by the organic matter content of the soil).

Table 3.2: Chemical vulnerability classes based on sorption behaviour and envelope equations.

Contaminant category	Vulnerability class	Soil property range defining vulnerability class					
		pH	S value	Clay	C	AI	Fe
Metal	High (H)	< 5	< 10	< 10			
	Moderate (M)	5-7	10-25	10-30			
	Low (L)	> 7	> 25	> 30			
Anionic and polar organic	High (H)	> 7	> 25	< 10	< 0.5	< 0.2	< 1
	Moderate (M)	6-7	10-25	10-30	0.5-1.5	0.2-0.8	1-3
	Low (L)	< 6	< 10	> 30	> 1.5	> 0.8	> 3
Non-polar organic	High (H)				< 1		
	Moderate (M)				1-3		
	Low (L)				> 3		

AVAP developed a spreadsheet programme: “AQUISOIL” (Aquifer Vulnerability Soil Assessment) (see Appendixes 19 and 24 ) to calculate chemical vulnerability classes based on laboratory data for the six soil properties. The manner in which chemical vulnerability classes are calculated is illustrated in Table 3.3. Following data entry (laboratory data) the chemical envelope equations calculate for metal and anionic or polar organic contaminants the expected sorption upper limit (y) from the value of each property (x). The property with the lowest sorption limit is then listed for information in the last column. It is this sorption limit which then determines whether the soil fits into a high, moderate or low vulnerability class (lower section of Table 3.3) for each of the three categories of contaminants (the third vulnerability, to non-polar organics, is calculated directly from the C classes in the Table).

The remainder of the proposed classification (and AQUISOIL spreadsheet) consists of superimposing additional criteria related to what can be termed hydraulic and climatic vulnerability as well as the thickness of the soil or regolith profile. As a first approximation, hydraulic attenuation classes can be created by considering (i) a permeability index, based on soil texture and whether or not a cemented layer or horizon is present (in this context the existing soil classification based on diagnostic horizons is invaluable, especially for morphological indications of restricted drainage and lateral discharge) and (ii) a leaching or recharge index calculated with one or other of the classical algorithms that take into account as many factors as possible (such as rainfall, surface runoff, profile storage, temperature, humidity, wind speed and transpiration potential of the vegetation cover) with as much frequency as the data allows (daily records being preferable to weekly, monthly or annual means). In the present scheme only three broad classes are assigned to the hydraulic (i.e. soil physical) and evaporative (i.e. climatic) vulnerability, and make use of depth in metres (minimum of 1m) as a denominator term. The latter effectively reduces vulnerability in direct proportion to the thickness of the soil profile or vadose zone, with maximum vulnerability

when depth is zero (i.e. groundwater and the soil surface coincide). The combination of chemical, hydraulic and climatic vulnerabilities is achieved by simple multiplication¹, which has the effect of producing, for different soils in different climatic contexts, a wide spread of values for overall vulnerability to a particular contaminant. The manner in which these physical factors are incorporated is illustrated in Table 3.4.

Table 3.3: Example of spreadsheet calculation of the chemical vulnerability classes to which a soil is assigned based on input values for six soil properties and employing the classification in Table 3.2*.

1. Chemical vulnerability					
Input values					
Al extracted with CBD		0.3	%		
Organic C		0.3	%		
Clay		18	%		
Fe extracted with CBD		1.18	%		
pH (CaCl ₂)		4.3			
S value: sum of basic cations		1.4	(cmolc/kg)		
Factor	Equation	r ²	Potential sorption (mg/kg)	Sorption limit (mg/kg)	Most restrictive property
Metals (e.g. copper)					
Clay	y = 663e ^{0.025x}	0.59	1034	267	S value
pH	y = 393x ² - 3563x + 8426	0.97	368		
S value	y = 132x + 82	0.97	267		
Anions (e.g. phosphate)					
Al	y = 1220x + 333	0.95	699	501	Fe
C	y = -35x ³ - 97x ² + 1088x + 299	0.82	616		
Clay	y = 76x ^{0.71}	0.77	595		
Fe	y = 198x + 267	0.91	501		
pH	y = 5222e ^{-0.33x}	0.69	1250		
S value	y = 1279e ^{-0.043x}	0.80	1205		
Chemical vulnerability class					No.
Metal pollutants			H		3
Anionic/polar organic pollutants			M		2
Non-polar organic pollutants			H		3

* A working spreadsheet, "AQUISOIL" is included on CD with this report (Appendix 19e ).

¹ Clearly there is no unique weighting that can be assigned to each of these three vulnerability scores in calculating overall vulnerability. Intuitively, however, their effects would appear to be multiplicative (i.e. there are interactions between them) rather than additive (which presupposes no interactions). For example, a low hydraulic rating means rapid solute movement and therefore less time available for chemical reaction, and *vice versa*. Another example would be the likelihood of inherently more rapid solute movement in clay soils of humid compared with arid environments (because of the type of clay mineral that develops in response to degree of weathering and the effect that this has on swelling, structure, porosity and colloid stability, and thus hydraulic conductivity).

Table 3.4: Continuation of the example in Table 3.3 illustrating the incorporation of physical parameters into vulnerability classification and the way in which groundwater vulnerability is calculated when data for more than one layer or horizon is available.

Thickness (d_i) of this layer (m):	5.0	Specify thickness of layer which chemical vulnerability has been calculated	
Total depth ($\sum d$) of all layers:	11.0		
2. Hydraulic vulnerability			
Restricting layer:	No	Specify "yes" if plinthite, dorbank, calcrete, clay or hard rock is present	
Hydraulic vulnerability class including texture:	No.		
Moderate	2		
Evaporative vulnerability:	arid	1	Specify arid, moderate or humid based on soil water balance
3. Overall vulnerability class			
Contaminant category	Single layer (v_i)^a	Weighted contribution to whole profile (v_p)^b	Profile-based vulnerability^c
Metal	0.22	2.73	$\sum v_{pm}/(1+\sum d)$
Anionic and polar organic	0.15	1.82	$\sum v_{pa}/(1+\sum d)$
Organic, non-polar	0.22	2.73	$\sum v_{po}/(1+\sum d)$
^a If C_m = chemical rating (1-3) for each material analysed, H = hydraulic rating (1-3) and E = evaporative rating (1-3), then overall rating (1-27) of a single layer is the product C_mHE . ^b Contribution is weighted according to thickness and vulnerability of each layer as follows: $v_p = v_i^{0.5} d_i / \sum d$ ^c For whole profiles or regolith consisting of more than one layer of material, profile-based vulnerability is the sum of the weighted contributions from each layer ($\sum v_p$) divided by $(1 + \text{total depth } (\sum d) \text{ in metres})$.			

In summary, the analysis of 170 soil materials revealed that the existing general purpose classification of South African soils is inadequate as a basis for predicting the attenuation of chemical contaminants. A new classification was developed which relates sorption to selected soil properties by means of chemical envelope equations based on segmented quantile regression. These envelopes predict the upper limit of contaminant sorption to be expected at a specified value of each soil property.

Soil classes for the retention of different categories of contaminants have been defined which, when combined with physical parameters (hydraulic and climatic), provide a basis for classifying soils and other regolith materials in terms of their contribution to groundwater vulnerability. Besides profile depth and site characteristics such as climate, the soil data required for the classification include clay, organic carbon, Al and Fe, pH and exchangeable cations.

Mills et al. (2006) have shown that to identify relational envelopes unequivocally require a sample population larger than one thousand. This could be regarded as a priority for future research since chemical envelopes offer an opportunity for classifying soils into different categories of pollutant attenuation (see Appendixes 19 and 24 for further details .

3.3 The EUZIT vulnerability assessment approach

The rating of the vadose zone (high, medium and low) is based on a combination of factors that contribute to the likelihood of contaminants reaching the saturated zone following the path of aquifer recharge. . The approach used, in order to improve DRASTIC, involved the description and quantification of these factors (Figure 3.3), as well as the provision of guidelines to assist in quantifying their relative importance. In addition, a database of values and descriptors related to the rating “I” (impact of the vadose zone) was included in a user-friendly, Excel-based Unsaturated Zone Index Tool (EUZIT) (Appendixes 20 and 24 ). The factors that serve as input to EUZIT are discussed individually in the following sections.

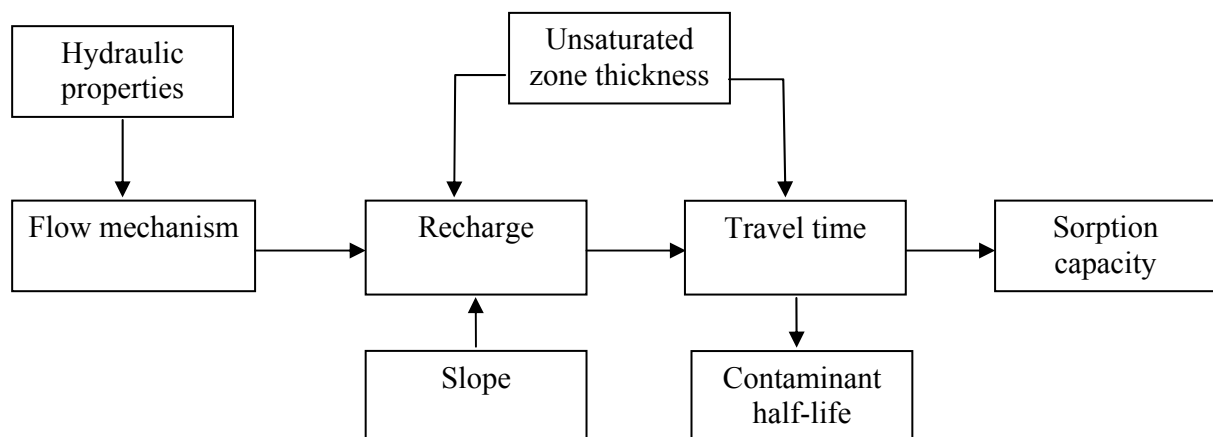


Figure 3.3: Relationship between the various factors that determine the attenuation capacity of the unsaturated zone.

3.3.1 Thickness of the unsaturated zone

It is important to assess the following when trying to describe the thickness of the unsaturated zone:

1. Whether the underlying aquifer is unconfined, confined, leaky or semi-confined; the most important aquifers for vulnerability assessments are of the unconfined and leaky aquifer types.
2. The type of regolith material (unconsolidated, consolidated, weathered, consolidated fractured or a combination)

Table 3.5 gives the relative influence of the thickness of the unsaturated zone based on the type of material constituting this zone. The values in Table 3.5 are included in the EUZIT software and they correspond to low, medium or high vulnerability impact of the unsaturated zone thickness.

Table 3.5: Unsaturated zone thicknesses, type of media and resulting impact on groundwater vulnerability.

Unsaturated zone medium		Thickness (m)		
Unconsolidated material	Gravel	> 50	30-50	0-30
	Clean sand	> 50	30-50	0-30
	Silty sand	> 30	15-30	0-15
	Silt	> 15	5-15	0-5
	Clay	> 5	> 2.5	> 0.5
Consolidated fractured medium		> 30	5-30	0-5
Leaky aquifers		> 30	5-30	0-5
Vulnerability impact				
		Low	Medium	High

3.3.2 Hydraulic properties

Estimation of soil hydraulic properties is important when trying to predict the fate and transport of chemicals in soil. Because of the difficulties and high labour costs associated with determining soil hydraulic properties, there is often a need to resort to estimating/modeling related soil parameters from other readily available data.

Unsaturated hydraulic functions are key input to numerical models. These functions may be either measured directly, estimated indirectly through prediction from more easily measured data based on quasi-empirical models, or approximated by using hydraulic data from similar soils or aquifer material. Typical values for hydraulic properties for most soil and aquifer material can be found in hydrology, hydrogeology and soil science textbooks or publications (e.g. Freeze & Cherry, 1979; Leij et al., 1996; and Halford & Kuniansky, 2002)

For the capacity of the entire sequence of the unsaturated zone to transmit water, the hydraulic conductance can be used. The hydraulic conductance is calculated with the following equation (Eimers et al., 2000):

$$C = \frac{K_{\text{unsat}} \times A}{L}$$

where K_{unsat} is the vertical hydraulic conductivity of the unsaturated zone, A (L^2) is the cross sectional area and L is the length of vertical flow or depth from land surface to the water table. K_{unsat} is difficult to estimate and is often substituted with saturated hydraulic conductivity (K_{sat}).

The ratings for various vertical hydraulic conductances are given in Table 3.6. The user selects the appropriate value and vulnerability impact of hydraulic conductance in the EUZIT software. If evidence of preferential flow exists, a high vulnerability impact is assumed to occur at vertical hydraulic conductances $> 1 \text{ m}^2 \text{ d}^{-1}$ (Table 3.6).

Table 3.6: Vertical hydraulic conductance and its impact on contaminant migration.

Flow mechanism	Vertical hydraulic conductance ($\text{m}^2 \text{ d}^{-1}$)		
Preferential			> 1
Matrix	< 45	45-9000	> 9000
	Vulnerability impact		
	Low	Medium	High

3.3.3 Flow mechanism (preferential and matrix flow)

Preferential flow paths are a major concern for predicting the vulnerability of aquifers to contamination. It is generally assumed that flow occurring through preferential flow paths will be fast (shorter travel times), resulting in lower sorption. The relationship between half-life and travel time will also become important, where longer travel times will favour attenuation. Dual-porosity and dual-permeability models for preferential flow in unsaturated structured media (macroporous soils, fractured rock) generally assumes that the medium consists of two interacting pore regions, the one associated with the macropore or fracture network, and the other with micropores inside soil aggregates or rock matrix blocks.

The formation of cracks on the soil surface due to swelling and shrinking of the clay fraction of the soil may have an impact on preferential contaminant transport. Swelling and shrinking especially occurs if smectitic clays are dominant in the soil. The impact of preferential flow is therefore deemed to be important for relatively shallow water tables. Where deeper water tables are present, the effect of soil surface cracks on groundwater contamination is negligible (Table 3.7).

Table 3.7: Percentage of smectitic clay fraction in the soil, depth to water table and resulting impact of groundwater vulnerability (low, medium or high).

Depth to water table (m)	% clay (predominantly smectites)		
	< 10	10-35	> 35
< 2	Low	High	High
2-5	Low	Medium	High
5	Low	Low	Low

In the absence of evidence of the clay content of soils, a simple evidence-based approach is suggested. Several indicators such as the presence of animal burrows, type of soils and the presence of vertical to sub-vertical fractures exposed near the surface provide evidence for preferential flow. The unsaturated zone chloride and soil moisture content profiling methods can be used to establish if preferential flow is occurring by inspecting the shape of the profile. The vulnerability impact of the different flow mechanisms is shown in Table 3.8. This is included in the EUZIT software.

Table 3.8: Dominant flow mechanism in the unsaturated zone and resulting impact on groundwater vulnerability.

Flow mechanisms		
Matrix only	Matrix flow and suspected preferential flow	Preferential flow
Vulnerability impact		
Low	Medium	High

3.3.4 Travel time

The velocity of leaching of a contaminant and the time it takes for it to move from the soil surface to the groundwater can be calculated using Darcy's equation and applying it to finite elements, assuming flow occurs under conditions close to saturation. The EUZIT software estimates travel time under conditions of natural infiltration and gross surcharging, using the equations of Foster and Hirata (1995).

Maxe and Johansson (1998) gave approximate velocities of water flow and travel times for soils under saturated conditions and unit gradient. The information is presented in Table 3.9

and it shows that, for example, a liquid spill reaches a relatively deep-lying water table in a gravel aquifer in less than a day. Macropore flow can result in shorter travel times.

Table 3.9: Approximate flow velocities and vertical travel times (Maxe and Johansson, 1998).

Soil	Water flow velocity	Vertical travel time			Ref.
		1 m depth	5 m depth	10 m depth	
Gravel	10-100 m h ⁻¹	< 1 h	< 1 h	< 1 h	1
Sand	10 cm d ⁻¹ - 1 m h ⁻¹	< 1 d	1 d – 1 mo	1 d – 1 a	1
Silt	1 cm – 1 m a ⁻¹	1 mo – 1 a	> 1 a	> 10 a	1
Clay	1 – 10 cm a ⁻¹	1 mo – 1 a			1
Sandy till	10 m a ⁻¹ – 1 m h ⁻¹	< 1 d	< 1 d – 1 mo	1 d – 1 a	2
Clayey till	10 cm – 100 m a ⁻¹	1 d – 1 mo	1 mo – 10 a	> 1 mo – 1 a	2
Peat	1 – 100 m a ⁻¹	> 1 d			1

The EUZIT software uses a simplification of the data of Maxe and Johansson (1998) to estimate travel time rating for various unsaturated zone media (Table 3.10). The table is included in the EUZIT software and the user can select the appropriate value and corresponding vulnerability impact of travel time. The table can be further expanded to include different thicknesses of the unsaturated zone.

Table 3.10: Unsaturated zone media type, travel time to water table and resulting impact on groundwater vulnerability for a 5 m thick unsaturated zone.

Unsaturated zone medium		Travel time		
Unconsolidated material	Gravel			< 1 h
	Clean sand		1 mo	1 d
	Silty sand	> 1a	< 1 a	< 1 mo
	Silt	> 0.5 a	0.5 a	< 1 mo
	Clay	>> 1 a		
Consolidated fractured medium		> 1 a	1 mo	1 h – 1 d
Vulnerability impact				
		Low	Medium	High

3.3.5 Recharge

Recharge estimation is probably the most difficult geohydrological variable to determine. Aquifer recharge is dependent on factors such as climate, geology (lithology and structures), geomorphology, vegetation, soil conditions and antecedent soil moisture. Recharge can either be diffuse and/or through preferential pathways. In the EUZIT software, recharge values can be estimated using four methods, namely the Guess estimate, the cumulative rainfall

departures (CRD), Earth and chloride mass balance (CMB) methods. These methods are applicable depending on the availability of data. The calculations are done in separate spreadsheets for each method. The ratings for recharge rate are given for various unsaturated zone thicknesses in Table 3.11, which is included in EUZIT.

Table 3.11: Unsaturated zone thickness, recharge and resulting impact on groundwater vulnerability.

Thickness (m)	Recharge (mm a ⁻¹)		
<5	0-1	1-5	> 5
5-30	0-5	5-10	> 10
> 30	0-10	10-100	> 100
Vulnerability impact			
Low Medium High			

3.3.6 Slope

A “Slope” sheet is included in the EUZIT tool. Troch et al. (2002) modeled the subsurface flow rates and soil moisture storage for nine hillslopes during free drainage at a constant depth of two meters. Zones with a concave topography produce more subsurface flow (Dunne, 1983; Troch et al., 2002) (Table 3.12).

Table 3.12: Slope, curvature and resulting impact on groundwater vulnerability.

Slope curvature	% Slope		
Convex	>12	2-12	0-2
Concave	>18	4-18	0-4
Vulnerability impact			
Low Medium High			

3.3.7 Sorption

The rating for impact of sorption on groundwater vulnerability can be determined in the AQUISOIL Excel spreadsheet (Appendix 19 ). The spreadsheet has as input six measurable soil properties and three groups of contaminants, namely (i) cationic (i.e. those ionic and mainly inorganic contaminants, chiefly metals, likely to have their sorption affected predominantly by the presence of negatively charged colloids); (ii) anionic (i.e. contaminants sorbing predominantly as ligands on positively charged surfaces or through covalent specific sorption; this class includes a range of polar organic substances in addition to inorganic anions); and (iii) non-polar organic substances, the retention of which is largely related, in

soils, to the content of organic matter. The chemical vulnerability classes for the three groups of contaminants are summarized in Table 3.2 (see Section 3.2). If soil properties such as pH, Clay, organic matter and exchangeable cation content are not available then samples must be taken before any realistic assessment can be made of soil and regolith contribution to chemical attenuation of contaminants.

3.3.8 Decay

Decay (degradation), expressed in terms of half-life, is related to organic contaminants subjected to physical (e.g. photolysis), chemical (e.g. hydrolysis) and biological (e.g. microbial) degradation. Half-lives of specific contaminants may vary by orders of magnitude depending on environmental factors (e.g. microbiological activity, pH, moisture, and temperature). Decay is strongly interlinked with sorption. A larger sorption will retard contaminant transport through the unsaturated zone and it will allow more time for contaminant degradation. The relation between decay and sorption and its potential impact on groundwater is summarized in Table 3.13.

Table 3.13: Contaminant persistence and sorption and its potential impact on groundwater.

Persistence	Sorption	Potential impact
Non-persistent	Low-moderate	Low
Non-persistent	Moderate-high	Low
Moderately persistent	Moderate-high	Moderate
Moderately persistent	Low-moderate	High
Persistent	Moderate-high	Moderate
Moderately persistent and persistent	Low-high	Site-specific conditions determine impact

A database of half-lives of contaminants as well as organic carbon partitioning coefficients (describing contaminant sorption) was compiled by Usher et al. (2004). Table 3.14 gives a general scheme for determining the vulnerability of an aquifer using information on the sorption capacity and half-life of contaminants.

Table 3.14: Unsaturated zone sorption capacity, contaminant persistence and resulting impact on groundwater vulnerability.

Sorption capacity	Half-life		
Low	< 1 h	< 12 h	< 24 h
Medium	1 d	1 – 15 d	15 – 30 d
High	1 – 15 d	15 – 50 d	> 50 d
Vulnerability impact			
Low Medium High			

3.3.9 Software application

The rating of the factors relevant to the attenuation of contaminants in the vadose zone was incorporated into a user-friendly Excel-based Unsaturated Zone Index Tool (EUZIT) (Appendix 25 ). A screenshot of the main menu of EUZIT is shown in Figure 3.4. The factors considered are those discussed in the previous section, namely the unsaturated zone thickness, hydraulic properties, flow mechanism, travel time, recharge, slope, contaminant sorption and degradation. If necessary, any of these factors can be disabled depending on site-specific conditions. The ratings for each factor are determined in sub-menus that include guidelines and theoretical descriptions. EUZIT also allows for a multi-layer vadose zone. The rating scores for each factor are combined in the main menu to yield the rating of the impact of vadose zone on groundwater vulnerability. The EUZIT programme draws the rating for sorption from the chemical vulnerability part of the AQUISOIL spreadsheet programme (see Section 3.2).

AVAP - Excel-based Unsaturated Zone Index Tool

Site:

Coordinates:

Layers:

General geology:

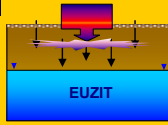
Rainfall: mm/yr

Area: m²

UNIT CONVERTER

All aquifers are vulnerable!!!

Shafick Adams
Nebo Jovanovic



EUZIT

Include

Parameter	Rating	Weight	Score
Thickness	☒	1	3
Hydraulic Properties	☒	1	3
Flow Mechanism	☒	3	9
Travel Time	☒	2	4
Recharge	☒	3	6
Slope	☒	2	2
Sorption Capacity	☒	2	4
Cont. Half-life	☒	3	9
Average		2.1	5.0

Average	Low	<2	<16	Index
5.0	Low	<2	<16	40
	Low-med	2-4	16-32	
	Medium	4-5	32-40	
	Med-high	5-7	40-56	
	High	>7	>56	

Figure 3.4: Screenshot of the main menu of the Excel-based Unsaturated Zone Index Tool (Appendix 26 ).

The vulnerability of an aquifer to contamination originating at the soil surface can be assessed using data that are readily available, that can be calculated or that can be estimated using the information provided in the database of EUZIT, based on the following step-by-step procedure (Figure 3.5):

1. The general slope of the area and the nature of the dominant hill slopes (convex or concave) is determined from available topographic maps. The rating for slope is then selected (Table 3.12).
2. The unsaturated zone thicknesses are determined using water level depths and national groundwater databases, as well as the nature of the unsaturated zone using borehole logs. A rating for the unsaturated zone thickness is then selected (Table 3.5).
3. The next step involves the calculation of the vertical hydraulic conductance using available data (Freeze and Cherry, 1979; Van Genuchten et al., 1991; Eimers et al., 2000; Lorentz et al., 2001; Halford and Kuniansky, 2002) or experimentally. The rating for hydraulic properties is then selected (Table 3.6). Models like RETC can also be used to calculate K values using pedotransfer functions. The “RETC program (Van Genuchten et al., 1991) uses the parametric models of Brooks-Corey and Van Genuchten to represent the soil water retention curve, and the theoretical pore-size distribution models of Mualem and Burdine to predict the unsaturated hydraulic conductivity function from observed soil water retention data.
4. The estimation of dominant flow mechanisms is done from tracer profiles, available borehole logs and geological information, as well as field observations. The rating of the flow mechanism component is determined (Tables 3.7 and 3.8).
5. The next step is the estimation of recharge using available information and any of the methods included in the EUZIT software (“Qualified Guess”, CBM, CRD, Earth). The rating for recharge is selected from Table 3.10.

6. Travel time is calculated using available data and any of the methods included in the software (flow velocity; Foster and Hirata, 1995). The rating for travel time is selected using Table 3.10.
7. Sorption and decay are defined from available information on soils and types of contaminants, experimentally or using compiled databases of contaminant properties (Usher et al., 2004). The rating for sorption is based on the AQUISOIL spreadsheet programme (Table 3.3; Section 3.2), whilst the rating for half-lives is selected from Table 3.14.

The process involved in determining groundwater vulnerability through EUZIT is graphically illustrated in Figure 3.5.

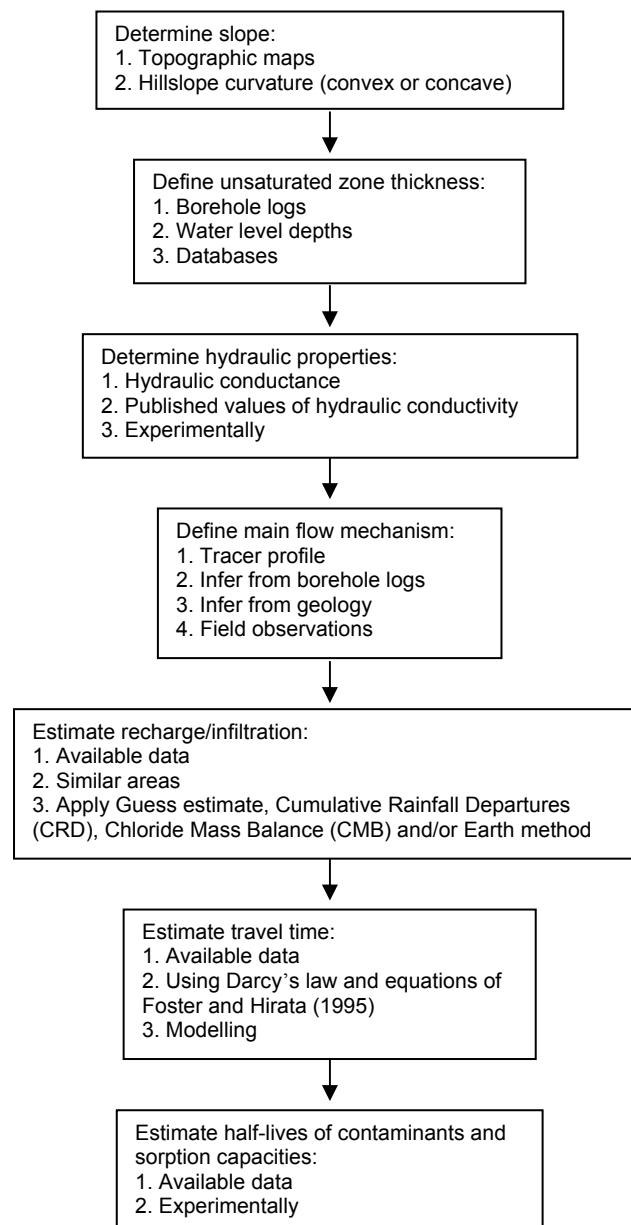


Figure 3.5: General scheme for determining the impact of the unsaturated zone on contaminant migration.

The EUZIT spreadsheet programme is underlain by a number of assumptions and limitations, which can be summarized as follows:

- The model embedded in the EUZIT programme is based on an index method and is not meant to calculate absolute values of environmental variables related to groundwater vulnerability. Therefore, the model is used for relative assessment between sites.
- The programme is mainly applicable to the local scale, although it can be easily linked to a GIS environment, where areas with different ratings can be delineated.
- Weighing of the eight factors is done subjectively.
- It is assumed that input data are available, reliable and representative of the scale to which the programme is applied. In particular:
 - Thickness of the unsaturated zone and layering depends on available and reliable data (e.g. borehole logs and water level depths).
 - The rating of hydraulic properties relies on the accuracy of hydraulic conductivity estimates. Ideally, unsaturated hydraulic conductivity data are required. Where these are unavailable, hydraulic conductivity is either estimated from other hydraulic properties, or is assumed to be equal to the value at saturation.
 - Flow mechanism rating depends on the availability and reliability of tracer profiles, borehole logs, geology or field observations. If there is evidence of preferential flow, the recommended rating of groundwater vulnerability is high.
 - The travel time calculations rely on the availability and reliability of input data, the accuracy of the equations of Foster and Hirata (1995) or any other model used.
 - Slope rating depends on the availability and reliability of topographic maps and measurements. Complex topographies need to be described by choosing one of the nine hillslope curvatures of Troch et al. (2002) as dominant.
 - Recharge rating depends on the availability and reliability of data. For comparative purposes, a number of methods are available to estimate recharge within EUZIT.
 - Soil analyses need to be available and reliable in order to determine the rating of sorption with AQUISOIL.
 - Half-life rating depends on the availability and reliability of degradation data for specific contaminants.

3.4 References

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CHAPTER 4:

VULNERABILITY ASSESSMENT OF THE SATURATED ZONE

Despite the widespread acknowledgement of the importance of processes within the saturated zone in determining the impact of contamination on groundwater, or in other words groundwater vulnerability, only few vulnerability assessment approaches include the buffering capabilities of the saturated zone. Margat, considered the originator of the term “groundwater vulnerability”, compiled the earliest groundwater vulnerability maps in France in the late 1960’s. His approach included a consideration of groundwater flow velocity as an indicator of the likely “persistence” of a contaminant in an aquifer (Margat and Suares-Parascandola, 1987). Andersen and Gork (1987) defined vulnerability as a function of the “cleansing” capacity of the soils and the restorative capacity of the aquifer. The U.S. National Research Council (1993) defined groundwater vulnerability as the “tendency for contaminants to reach a specified position in the groundwater system after introduction at some location” (NRC, 1993 in Vrba and Zaporozec, 1994). Key physical parameters which determine groundwater vulnerability in their approach include lithology, thickness, effective porosity, groundwater flow direction, age and residence time of water. Generally, the residence time of a contaminant in groundwater and the distance that it travels in the aquifer are considered important measures of vulnerability.

4.1 Two approaches for determining saturated zone vulnerability

Two approaches were developed for both inorganic and organic contamination to determine saturated zone vulnerability for two important aquifer types in South Africa, considered at present to be particularly vulnerable to pollution. These are:

- Coastal primary aquifers, composed primarily of Recent/Quaternary sediments, and
- Dual porosity aquifers (mixed fractured/porous) aquifers developed in the weathered zone overlying sedimentary or igneous rocks.

Geochemical characteristics of the two types of aquifers are described in the next section (Section 4.2; see also Appendixes 4 and 7 ). The first approach is discussed in Section 4.3 and comprises the following steps (see also Appendixes 7, 10 and 18 ):

1. Simulation of the chemical evolution of the naturally-occurring groundwater, based on a geochemical description of the aquifer and probable reactions of recharge water with minerals and organic matter in the aquifer. The aim of this step is to achieve a reasonable geochemical simulation of the aquifer.

2. Modeling of the injection and reactive transport of the contaminant cocktail at each site, directly into the aquifer, discounting the role of the soil and unsaturated zones in protecting the aquifer.
3. Comparison of aquifers and contaminants in terms of (a) how far from the source contaminants exceed a preset concentration level, at a given time and (b) for what period of time contaminant concentrations exceed that set concentration, at a given distance from the source.

A second approach for determining saturated zone vulnerability is more generic and is based on the analytical equations for mass transport such as the Domenico equation and is discussed in Section 4.4.

4.2 Geochemical characteristics of primary and dual-porosity aquifers

4.2.1 Coastal primary aquifers

Geochemical environment

Coastal primary aquifers with the highest groundwater yield potential are predominantly unconsolidated sands. Shell fragments make up a significant proportion of the sand-sized fragments, with the remainder being quartz and possibly heavy mineral oxides. Clay minerals may be present, either widely disseminated or present as discrete lenses and horizons. In general, the clay content of a coastal primary aquifer of good groundwater potential does not exceed 20%.

Recharge water quality

In coastal areas it is possible to generalise that the dissolved ion concentration in rainwater is derived from sea salt aerosols. In essence, coastal rainwater is highly dilute seawater. Some recent data from analyses of rainwater collected at for instance Cape Point illustrate this:

Table 4.1: Comparison between seawater at high dilutions and rainwater collected at Cape Point.

milliequivalents/litre or unitless	Seawater	Seawater diluted 500x	Seawater diluted 1000x	Cape Point rainwater (Brunke, pers. comm., 2004)
pH	8.2	-	-	5.5-6.5
Ca ²⁺	20.6	0.041	0.020	0.035
Mg ²⁺	106.3	0.21	0.11	0.106
Na ⁺	468.4	0.94	0.47	0.854
K ⁺	10.2	0.020	0.010	0.036
NH ₄ ⁺	0.002	3.3 x 10 ⁻⁶	1.7 x 10 ⁻⁶	0.0
Cl ⁻	545.9	1.1	0.54	0.853
NO ₃ ⁻	0.005	9.4 x 10 ⁻⁶	4.7 x 10 ⁻⁶	0.040
SO ₄ ²⁻	56.5	0.11	0.056	0.081
Total Alkalinity	2.3	-	-	0.116 (est.)

The rainwater is close to dilute seawater in respect of Ca, Mg, Na, Cl, K and SO₄ concentrations. Alkalinity and pH in rainwater are controlled by the concentration of dissolved atmospheric CO₂. The additional NO₃ observed at Cape Point probably originates from terrestrial dust.

Redox conditions

In unconfined, shallow coastal aquifers, redox conditions are controlled by the diffusion of oxygen into the aquifer from surface and the presence of reducing agents, especially organic matter. Oxygen diffusion depends on the permeability of the unsaturated zone, and depth below the water table – in less permeable media and at greater depths in the aquifer, anoxic conditions are likely. Carbon input to the aquifer will depend on the productivity of the surface and soil ecosystems. Sparsely vegetated dune fields will generate little soluble organic matter that can be transported through the unsaturated zone and into the aquifer.

Processes and reactions

Evaporative concentration

On average, evapotranspiration rates exceed precipitation rates in most coastal regions of South Africa. But recharge takes place during wet periods when precipitation temporarily exceeds evapotranspiration. This recharge water will encounter and dissolve salts precipitated in soil and the unsaturated zone during drier periods. The net effect is that recharge water has the composition of concentrated rainwater. The concentration factor is the inverse of the recharge factor. For example, if recharge is 5% of precipitation, the concentration factor would be 20, i.e., the dissolved concentrations of conservative solutes in groundwater are 20 times that of rainwater.

Oxidation of organic matter

Dissolved organic matter will be oxidised by oxygen and other oxidising agents (e.g. nitrate and sulphate) to CO₂. CO₂ dissolves in water to generate acidity and alkalinity.

Dissolution & precipitation of carbonate minerals

Shell material, mainly aragonite and calcite, tends to dissolve in the acidic water with relatively low concentrations of dissolved calcium. This process raises the concentration of calcium relative to magnesium (which is higher than calcium in marine-derived recharge water). The groundwater tends toward equilibrium with calcium and magnesium carbonate minerals, principally calcite and dolomite. The actual compositions of these minerals are probably intermediate between calcite and dolomite, as it is well known that magnesium-rich calcite does occur, while dolomite formation requires rather high Mg:Ca ratios.

Cation exchange

A clay content of 20% places an upper boundary on the aquifer sediment's cation exchange capacity (CEC). Assuming a clay with a CEC of 100 millequivalents/kg (Drever, 1997), the average CEC of the aquifer is 20 meq/kg. If the aquifer has a porosity of 20% and the matrix S.G. = 2.0, each litre is in contact with 8 kg of aquifer material $\times$ 200 meq/kg = 160 meq per litre. In more dilute water, divalent ions (Ca^{2+} and Mg^{2+}) will tend to displace monovalent ions (Na^+) from exchange sites. At higher concentrations the reverse takes place. In general, cation exchange provides an important control of groundwater's ionic composition.

Modelling natural groundwater composition

The compositional evolution of groundwater can be simulated, using the geochemical model PHREEQC-2 (Parkhurst and Appelo, 1999), in 3 steps (Figure 4.1):

1. *Evaporative concentration & equilibration with carbonates*
2. *Addition of organic matter and lower O_2 concentration*
3. *Anoxic conditions & additional organic matter*

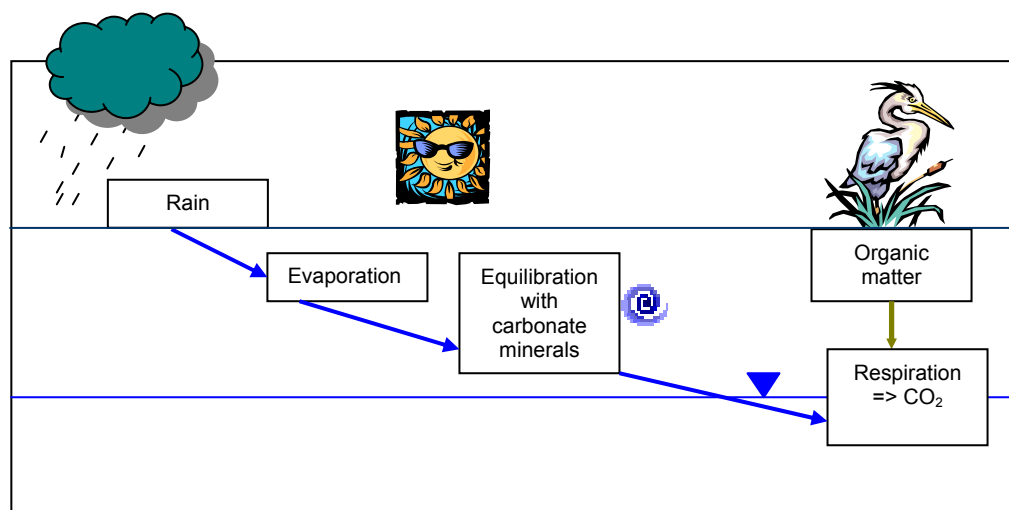


Figure 4.1: Components of the model of the chemical evolution of groundwater in a coastal aquifer.

The steps represent the processes taking place at increasing depth, from surface (1), through the soil and vadose zone (2), to the saturated zone (3). Steps 2 and 3 can be simulated with (2 & 3a) and without cation exchange capacity (2 & 3b) in the aquifer. The composition of the water at each step is presented in Table 4.2.

Table 4.2: Simulated compositions of recharge and groundwater in coastal primary aquifers.

meq/litre or unitless	Rainwater (seawater diluted 1000x)	Step 1: Concentrate (20x) & equilibrate with calcite & dolomite	Step 2: Add organic matter & lower pO ₂	Step 3a: Reduce pO ₂ to zero & add more OM	Step 3b: With cation exchange in steps 2 & 3, CEC = 0.2 eq/litre	Cape Flats aquifer – near Coastal Park landfill
pH	5.5	8.1	7.1	7.1	7.1	7-8
Ca ²⁺	0.02	1.6	2.9	3.0	2.6	5-7
Mg ²⁺	0.11	1.4	2.5	2.5	2.2	3-5
Na ⁺	0.47	9.4	9.4	9.4	10.7	8-25
K ⁺	0.01	0.2	0.2	0.2	0.2	0.25-0.75
Cl ⁻	0.54	10.8	10.8	10.8	10.8	10-30
NO ₃ ⁻	4.7 x 10 ⁻⁶	10 ⁻⁴	0.3	0.08	0.08	0-0.03
SO ₄ ²⁻	0.056	1.1	1.1	1.1	1.1	0.2-0.4
Total Alkalinity	10 ⁻³	0.8	5.4	5.6	5.7	6-10


 SIMULATED OBSERVED

4.2.2 Dual-porosity, weathered zone aquifers

These aquifers are found at relatively shallow depths throughout South Africa, in various geological units. They represent the uppermost aquifer, and may not necessarily provide the best groundwater yield or quality. However, being closest to most anthropogenic contamination they are more readily contaminated than deeper aquifers. With bypass or preferential flow, however, contamination of deeper aquifers or surface water bodies could also take place.

Geochemical environment

The rock types which support these aquifers are diverse. Weathering of relatively soluble minerals (especially olivine, pyroxene and feldspar) is an important source of the commonly observed dissolved metal ions in groundwater.

Recharge water quality

In general, the further inland, the less pronounced the marine signature in rainwater, and the lower the concentrations of dissolved ions. The concentrations of calcium, magnesium, nitrate and ammonium typically exceed those of sodium and chloride, with calcium being dominant. Sulphate, nitrate and acidity increase close to urban and industrial areas, caused by acid emissions from fossil fuel combustion.

However, the dissolved ion concentrations are very low in inland rain, generally less than 0.1 meq/litre. Unless the rainwater is particularly acidic or has an unusual chemical signature, the chemical processes occurring below the surface in this type of aquifer probably exert more control on groundwater composition than rainwater quality. Recharge water can be treated as

a very dilute solution (0.05 millimolar) of calcium chloride and calcium bicarbonate, in equilibrium with atmospheric CO₂.

Redox conditions

Key controls are the permeability of the vadose zone and aquifer to oxygen, depth of the water table, inputs of organic matter and the presence of reduced species, such as sulphides, and presence of alternative electron acceptors in the absence of oxygen in the aquifer matrix.

Processes and reactions

Evaporative concentration and the oxidation of organic matter

These processes are discussed in Section 4.2.1 and apply equally in weathered zone aquifers.

Mineral dissolution and precipitation

Dissolution of primary minerals, especially pyroxene and feldspar in the South African context, is the main source of the metal ions in groundwater – calcium, magnesium, sodium, potassium and iron. These minerals weather to secondary minerals, especially clay minerals and micas, which are less soluble but impart increased cation exchange capacity to the aquifer.

Cation exchange capacity

Assuming a clay with a CEC of 200 meq/kg, an aquifer clay content of 25%, and 25% porosity, and an aquifer matrix S.G. of 2.0, the likely upper limit of CEC in these aquifers is 0.3 equivalents/litre.

Modelling natural groundwater composition

Natural groundwater can be simulated in two steps:

1. *Evaporative concentration*
2. *Equilibration with primary minerals and elevated CO₂ concentration*

The initial recharge water is concentrated 50 times, to simulate the effect of high levels of evapotranspiration which result in a low percentage recharge (1-2%). The minerals chosen are diopside, a calcium-magnesium pyroxene, and albite, a sodium feldspar. These are chosen for convenience, as chemical thermodynamic data on these minerals is readily available. The partial pressure of CO₂ is set at 3.5%, or 100 times atmospheric pressure, to simulate the effect of the respiration of soil biota. The conceptual model is illustrated in Figure 4.2.

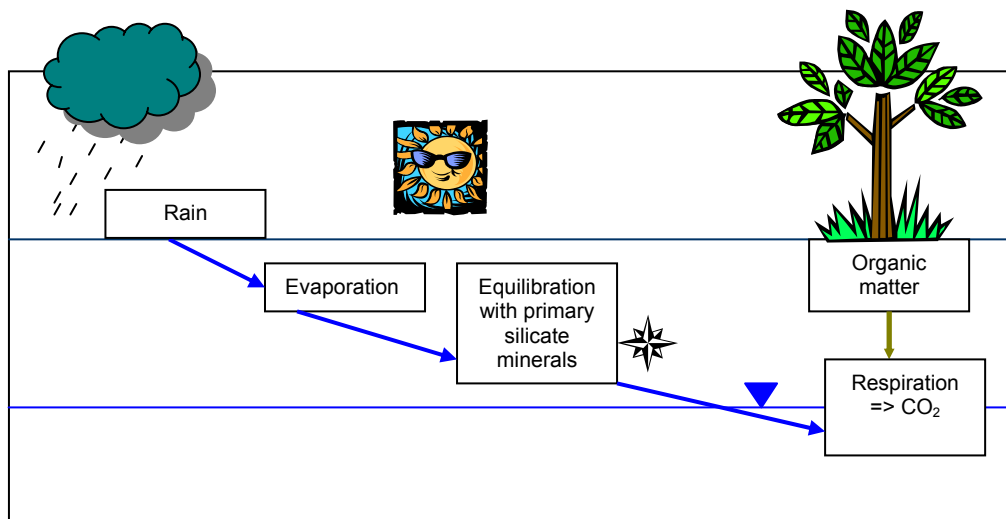


Figure 4.2: Components of the model of chemical evolution of groundwater in a weathered zone.

In a third step, cation exchange sites are equilibrated with the resulting solution. The resulting exchange site composition will be the initial state for the contaminant transport modelling.

The results of the modelling, i.e. simulated weathered zone groundwater composition, with ranges of actual groundwater composition from a weathered zone aquifer at Secunda for comparison, are shown in Table 4.3.

Table 4.3: Simulated composition of recharge water and groundwater in an inland, weathered zone.

Meq/litre or unitless	Recharge	Step 1: Concentrate (50 x)	Step 2: Equilibrate with Ca-Mg pyroxene and Na-feldspar at 3.5% CO ₂	Step 3: Allow calcite precipitation & equilibrate with cation exchange	Karoo Supergroup aquifer, Secunda (Sasol, 2002)
pH	5.7	5.7	7.4	6.9	7.2-8.5
Ca ²⁺	0.1	5.0	12.0	3.3	2.8-7.0
Mg ²⁺	0	0	7.0	1.8	2-4
Na ⁺	0	0	0.002	0.005	2.5-7.0
Cl ⁻	0.1	5.0	5.0	5.0	0.5-9.9
Alkalinity	10 ⁻¹⁰	10 ⁻⁸	14.0	5.2	4.2-10.1

4.3 Saturated zone vulnerability - Geochemical and reactive transport models

4.3.1 Inorganic contaminant sources

Three classes of contaminant mixtures or “cocktails” were considered for assessing inorganic contamination: industrial effluents, with high levels of nutrient and trace elements, domestic landfill leachate and acid mine drainage (see Table 4.4). The methodology for determining saturated zone vulnerability for inorganic contaminants in terms of spatial impact and persistence of a contaminant and using geochemical and reactive transport models is discussed below and is followed by a summary of findings on vulnerability for the three contaminant cocktails for both aquifer types.

Table 4.4: Composition of inorganic cocktails.

Variable	Landfill leachate (Novella <i>et al.</i> , 1999)	Industrial Effluent (Sasol, 2002)	Acid Mine Drainage (simplified)
	Millimolar		
pH	7-8	5-8	0.01
Ca	5	3	
Mg	5	4.5	
Na	45	5	
K	25	3.5	
Cl	92	0.2	
NO ₃ ⁻	1	5	
NH ₄ ⁺	55	8	
SO ₄ ²⁻	1	3.5	10500
Total Alkalinity	50	2	
Pb			5200
Fe			3000

Spatial impact and persistence

Each aquifer type was modelled with PHREEQC-2 (Parkhurst and Appelo, 1999) as a column of 12 distance units (cells), with identical physical properties, but different geochemical properties as described in the Section 4.2. The contaminant mixture is injected into the aquifer in two ways – either from a continuous source or from an instantaneous pulse, followed by flushing with uncontaminated groundwater. The change in chloride concentration (as conservative species) with time (in various units) at the outflow of the modelled aquifers illustrates the difference between the two modes of injection (Figure 4.3).

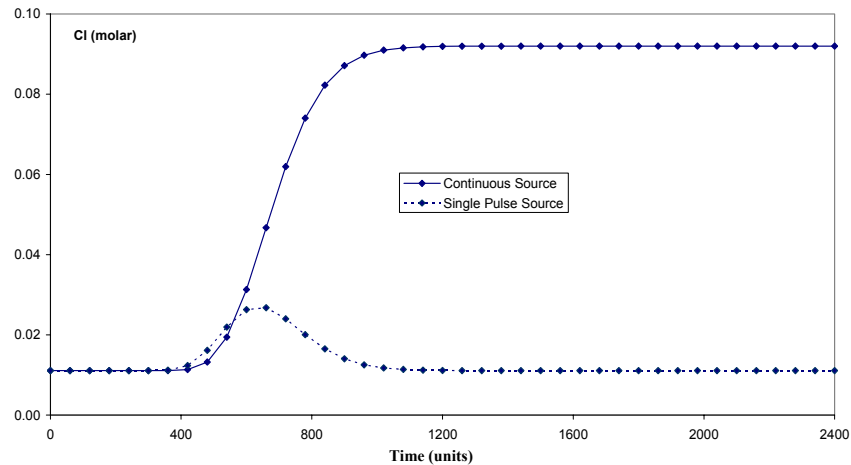


Figure 4.3: Chloride concentration vs. time at the outflow point of the simulated aquifers, with continuous and single-pulse sources of contaminant mixtures.

Spatial component of vulnerability

A continuous source of the contaminant (mixture) is injected into the aquifer. At a certain time (for example, the time to a breakthrough of a conservative solute such as chloride at a specific distance from the source), a snapshot is taken of the concentration of the contaminant of interest along the traveled distance or flow path. The distance (or in modelling terms: cell number) furthest from the source in which the concentration exceeds a reference level (e.g. 5% of the input concentration, or natural background), is defined as the spatial impact. Figure 4.4 is an example of the spatial impact of contamination for the two aquifer types considered. Illustrated are the changes along a flow path (distance in cells) of fluoride from a continuous injection of industrial effluent at the breakthrough time of chloride (=360 time units at the end of the flowpath). The fluoride concentration in the primary aquifer is generally higher along the flowpath. Note that the fluoride concentration has reached 5% of the injection concentration at a greater distance from the source (cell 6) than in the weathered zone aquifer (cell 5). The primary aquifer has in this case a slightly higher spatial vulnerability with respect to fluoride.

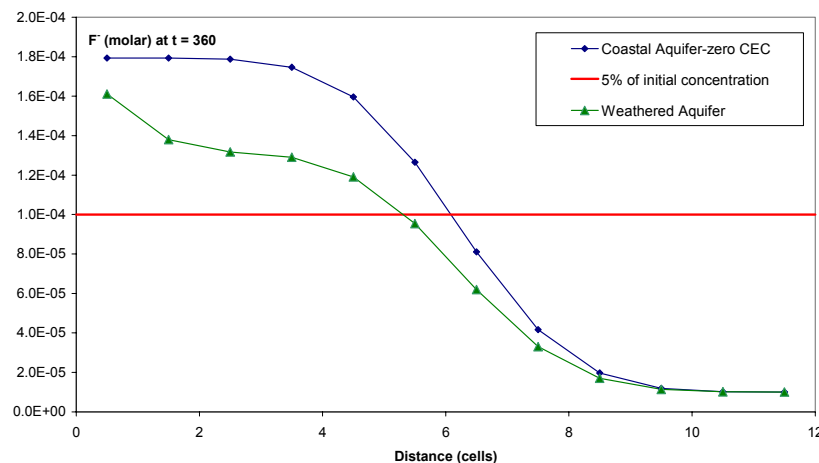


Figure 4.4: Fluoride concentration against distance in the simulated coastal and weathered zone aquifers at time = 360 units (Appendix 7 ).

Temporal component of vulnerability (persistence)

Using the scenario of a pulse of contaminant mixture, followed by flushing, the residence time or persistence of a contaminant in different aquifers can be compared. Persistence is defined as the time it takes for the concentration of the contaminant at a fixed distance in the aquifer from the source to fall below a certain level, say for instance 5 % of the initial (input) concentration. Figure 4.5 is an example of the persistence to contamination for the two aquifer types considered. Illustrated are the changes in time of the pH and lead concentration from an injection of a pulse of acid mine drainage at a specific distance from the source in the aquifer. It can be seen that the lead concentration persists above the background level (about 1.5 micromolar) for about 1200 units of model time from the start, in the coastal (primary) aquifer, against about 1000 time units for the weathered zone (dual porosity) aquifer. In this case, the primary aquifer can be considered more vulnerable (by about 20%) than the weathered zone aquifer.

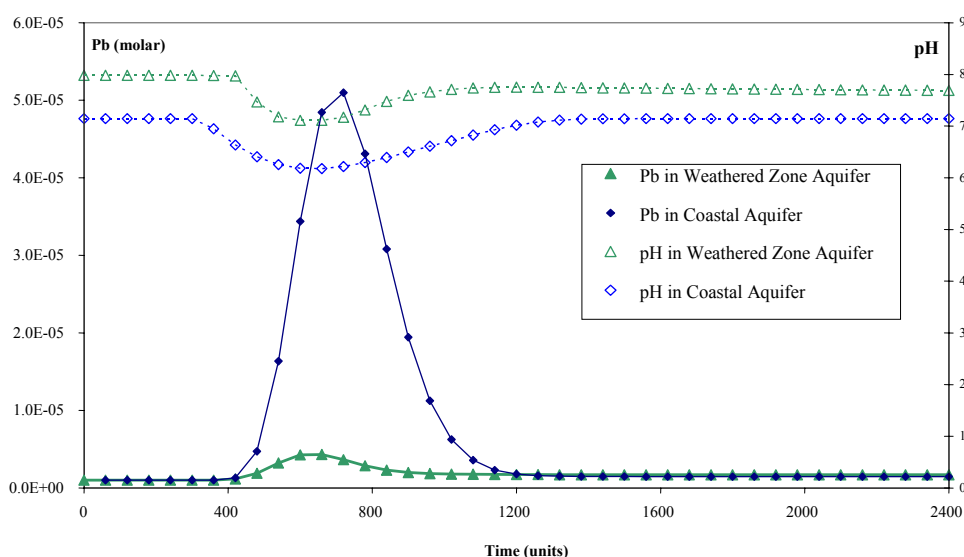


Figure 4.5: Lead concentration (moles/litre) and pH vs. time at specific distance from the source in coastal and weathered zone aquifers (Appendix 7 ).

Saturated zone vulnerability indices

The geochemical model PHREEQC-2 (Parkhurst and Appelo, 1999) was used to derive generic vulnerabilities, assuming identical physical properties, of both aquifer types to three sources of dissolved inorganic contaminants. Table 4.5 shows a matrix of values for the spatial and temporal indices which facilitates a comparison of vulnerability between the various options.

In the primary aquifer for example, the spatial impact of ammonium is greater than that of fluoride. Thus, the primary aquifer is more vulnerable to the landfill leachate than for the industrial effluent. If we compare the primary with the dual porosity aquifer, the persistence to both contaminating sources is higher for the dual porosity aquifer, whereas for the spatial impact the opposite is observed. In other words, regarding the contaminant sources of landfill leachate and industrial effluent, the dual porosity aquifer is more vulnerable in terms of persistence than the primary aquifer but less vulnerable in terms of spatial impact.

Table 4.5: Saturated zone vulnerability in coastal (primary) and weathered zone aquifers (see Appendix 7 ).

Source Type & Contaminant of Concern	Aquifer Types	
	Unconsolidated Primary Aquifer (Cape Flats)	Dual Porosity (primary/fractured) Aquifer (Ecca Group, Karoo Supergroup, Secunda)_
Landfill leachate AMMONIUM	Major controls: dispersive processes	Major controls: cation exchange and dispersive processes
	Spatial impact: 9 (in cells) Persistence: 1000 (in time units)	Spatial impact: 5 Persistence: 7000
Industrial Effluent (Secunda type) FLUORIDE	Major controls: Precipitation of calcium fluoride and dispersive processes	
	Spatial impact: 6 Persistence: 1300	Spatial impact: 5 Persistence: 1600
Acid mine drainage with trace metals LEAD & ACIDITY	Major controls: Precipitation of lead hydroxides and dispersive processes	Major controls: Precipitation of lead hydroxides, cation exchange and dispersive processes
	Spatial impact: 2.5 Persistence: 1200	Spatial impact: 3.5 Persistence: 1000

Where one is concerned about the potential impacts on groundwater in the area surrounding an industrial plant, for example, a high *spatial impact* score indicates a high probability that contaminated groundwater will move off-site before corrective action is taken.

When the concern is about the long-term impacts on groundwater of some activity, for example an ore refinery at a mine which has a limited lifespan, a high *persistence* score indicates a high probability that groundwater at the site will remain contaminated after the polluting activity has ceased.

In addition, it is possible to compare the vulnerability of the aquifer to different contaminants in the same, or different, contaminant mixtures. For example, in the coastal aquifer, the spatial impact of ammonium is greater than that of fluoride.

It should be noted that vulnerabilities of both aquifer types, based on realistic spatial and temporal scales (i.e. using their unique physical properties) are derived from the linking of PHREEQC-2 (Parkhurst and Appelo, 1999) with a single or multi-species groundwater flow/transport model such as MT3DMS (Zheng and Wang, 1999). This has been done for the case of Goedeheop at Secunda (see Chapter 6 and Appendix 10 .

4.3.2 Dissolved organic contaminant sources

A similar methodology as applied to inorganic contamination was adopted for evaluating the spatial impact and persistence of dissolved organic contaminants in the saturated zone (Appendix 18 ). Previous research on the most likely organic contaminants in South African aquifers (Usher et al., 2004) have indicated that petroleum hydrocarbons and chlorinated solvents of industrial effluents are two of the most likely contaminants expected.

Modelling reactive transport

The following models: PHT3D (Prommer, 2003), BIOPLUME III and the LNAPL Guide (American Petroleum Institute, 2004) were used for simulating reactive transport of BTEX (Benzene, Toluene, Ethylbenzene and Xylene; considered representative of petroleum hydrocarbons), and the BIOCHLOR code (Aziz et al, 2000) for chlorinated ethenes. Processes accounted for in the simulations included biodegradation with and without volatilisation and sorption.

PHT3D is a multicomponent transport model for three-dimensional reactive transport in saturated porous media. It incorporates [MT3DMS](#) for the simulation of three-dimensional advective-dispersive multi-component transport and the geochemical model [PHREEQC-2](#) for the quantification of reactive processes.

BIOPLUME III is a two-dimensional model for simulating the biodegradation of hydrocarbons in groundwater. The model simulates both aerobic and anaerobic biodegradation processes in addition to advection, dispersion, sorption and ion exchange. The model was used to evaluate the persistence of BTEX.

The Interactive LNAPL Guide (American Petroleum Institute, 2004) is an easy-to-use electronic information management system to provide understanding and tools for evaluating LNAPL mobility and recoverability. The Guide was used to simulate the persistence and maximum downgradient movement of the benzene contaminant in the aquifer. It accounts for parameters such as volatilisation, biodegradation, water table fluctuations, and retardation. The guide is somewhat limited in that it considers only a constant contaminant spill, without taking into account possible dilution from recharge.

The BIOCHLOR code was used to model the progressive dechlorination and degradation of chlorinated ethenes to enable comparison with a BTEX pollution plume. Maximum rates of degradation would occur under reducing anaerobic conditions.

Saturated zone vulnerability indices

Retardation was found to play an important role in the degradation of compounds. The simulation of benzene with and without sorption showed an immense difference. A small increase in the fraction of organic carbon resulted in a drastic decrease in plume extent. In reality the aquifer will have some organic carbon and therefore sorption will play a significant role in determining aquifer vulnerability. With regards to biodegradation, the depletion of contaminant concentrations was found to be far less pronounced closer to the source and volatilisation would drastically reduce the persistence of a contaminant.

The vulnerability of dissolved organic contaminants needs at least to take the nature of the spill, the type of release and the composition of the NAPL into account, together with the site implications for each parameter. The chlorinated ethane simulation indicated the importance

of defining the geochemical conditions on site, and the limitations of defining vulnerability for organics as a generalization. The spatial impact was generally found to be highest for Benzene whereas its persistence is relatively lower.

4.4 Saturated zone vulnerability – Generic approach

An alternative to the numerical modelling or often complex reactive transport models as described in Section 4.3 would be a generic approach to determining saturated zone vulnerability. Generic approaches generalise the transport of a contaminant by an analytical equation. Examples are the Ogata-Banks approximation and the Domenico mass transport equation (Domenico, 1987). The generic approach is appropriate for screening. The limitations are the correct assumptions to be made by practitioners and the required info for the contaminants of concern. The reactive transport modelling approach would be theoretically the most correct but for integration into a multi-disciplinary versatile approach, the level of complexity may be too great for general implementation. The Domenico analytical equation is proposed for the generic approach due to its versatility and widespread use in many attenuation assessment tools (e.g. in BIOCHLOR; Aziz et al., 2003), and the fact that degradation and retardation can be included.

Note that the development/adoption of a generic approach was only proposed recently hence only a theoretical framework as well as a simplified guide are presented in the following sections.

4.4.1 *Domenico mass transport equation*

The Domenico analytical equation is based on the advection-dispersion partial-differential equation for organic contaminant transport processes in groundwater as described below (Domenico and Robbins 1985):

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - v \frac{\partial C}{\partial x}$$

where:

C - contaminant concentration in groundwater (mg/L),

t - time (day),

v - groundwater seepage velocity (m/day),

x, y, z - coordinates to the three dimensions (m),

D_x, D_y, D_z - dispersion coefficients for the x, y, z dimensions (m²/day), respectively.

To solve this equation analytically, under conditions of the steady-state source and finite continuous source dimension with one-dimensional groundwater velocity, three dimensional

dispersion, and a first order degradation rate constant, the analytical solution can be expressed as (Domenico, 1987):

$$\frac{C_x}{C_0} = \exp\left\{\frac{x}{2a_x}\left[1 - \left(1 + \frac{4\lambda a_x}{v}\right)^{\frac{1}{2}}\right]\right\} \operatorname{erf}\left[\frac{Y}{4(a_y x)^{\frac{1}{2}}}\right] \operatorname{erf}\left[\frac{Z}{4(a_z x)^{\frac{1}{2}}}\right]$$

where:

C_x - contaminant concentration in a downgradient well along the plume centreline at a distance x (mg/L),

C_0 - contaminant concentration in the source well (mg/L),

x - centerline distance between the downgradient well and source well (m),

α_x , α_y , and α_z - longitudinal, transverse, and vertical dispersivity (m), respectively,

λ - degradation rate constant (1/day),

$\lambda = 0.693/t_{1/2}$ (where $t_{1/2}$ is the degradation half-life of the compound).

v - Contaminant velocity in groundwater (m/day),

Y - Distance from centerline of source (m),

Z - Vertical distance from groundwater surface to measurement point (m),

erf - error function,

$\exp$ - exponential function.

It is important to note that the term R is the velocity of the contaminant not the advective transport and includes the retardation term:

$$R = V/V_c = 1 + \rho_b k_d / \theta$$

The degree of retardation depends on both aquifer and constituent properties. The retardation factor is the ratio of the groundwater seepage velocity to the rate that dissolved chemicals migrate in the groundwater.

The Domenico analytical equation assumes:

- A finite source dimension,
- A steady state source,
- Homogeneous aquifer properties,
- One dimensional groundwater flow,
- First order degradation rate,
- Contaminant concentration estimated at the centerline of the plume,
- Molecular diffusion based on concentration gradient is neglected,
- No retardation (e.g., sorption) in the transport process.

Understanding model assumptions is crucial to simulate the transport process for a specific contaminant in groundwater. The Domenico equation assumes a vertical plane source oriented perpendicular to groundwater flow to simulate the release of contaminants to moving groundwater. In addition, the Domenico solution accounts for the effects of one-dimensional advective transport, three-dimensional dispersion, adsorption, and first-order decay.

4.4.2 Saturated zone vulnerability indices

The steps for determining saturated zone vulnerability could be as follows:

- Select a consistent distance away from the source to be assessed. A distance of 150 m may be used to fall in line with early efforts by de Lange (1999) to determine protection zones in South Africa.
- Select a period of contamination to be assessed. Alternatively a steady-state approach, using the steady state Domenico equation may be used.
- Input the site-specific conditions and assess the plume migration of conservative species at the specified time and distance.
- Establish consistent assessment criteria. Following the approaches outlined in Demona (Kalsch et al, 2004), the percentage of input concentration can be used to assess the aquifer's attenuation capacity or vulnerability. The same scoring and classification as used in the Excel EUZIT Tool for the unsaturated zone (Chapter 3) is suggested.
- From this approach the non-specific or general vulnerability can be obtained. This can give an "intrinsic" overall vulnerability of the system.
- The "specific" vulnerability can be determined when selected contaminant's properties within the aquifer are included. In this way, retardation and degradation can be included and a truer measure of the vulnerability can be assessed. In cases, where it is possible to predict the concentration/load of the contamination entering the aquifer from the unsaturated zone, as is possible with UGIf (Chapter 5), the specific vulnerability can be determined as a function of the percentage or, if preferred, as comparison to defined water quality criteria.

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CHAPTER 5:

GIS-BASED GROUNDWATER VULNERABILITY ASSESSMENT

A Geographical Information Systems (GIS) is well suited to carrying out analysis of spatially referenced layers of information. The ability to convert data layers into raster (cell-based) data sets can facilitate the rapid achievement of a final result of a groundwater vulnerability assessment. GIS enables the compilation of vulnerability maps combined with other infrastructural information so that the results can be easily related to by planners and decision makers.

5.1 AVAP's GIS-based approaches

Index and process-based approaches to vulnerability assessment can be relatively easily incorporated in a GIS. Both approaches were applied in AVAP.

The starting point for the *index* approach was the DRASTIC model (Aller et al., 1987) which is often incorporated in a GIS using the concept of georeferenced raster layers and “layer calculations”. The raster layer approach facilitates the assignment of ratings and weightings. Algorithms can easily be repeated as new or more detailed data sets are obtained, or if ratings and weightings need to be adjusted. Initial efforts of AVAP focused on incorporating the various zones, i.e. the soil, intermediate and saturated zones into a modified DRASTIC which was called the ReSIS model (see Appendix 12 ). With the research progressing the intermediate zone was no longer treated independent from the soil zone and hence another model, EUZIT, was developed to assess vulnerability of the unsaturated zone as a whole (see Chapter 3). Lumping vulnerability indices of the unsaturated and saturated zones was discarded as to enable decision-makers to better understand (a) the likelihood of contaminants arriving at the water table (unsaturated zone vulnerability) and (b) the spatial impact and persistence of contaminants in the saturated zone (saturated zone vulnerability).

EUZIT was later integrated in a GIS to assess the variation in groundwater vulnerability across an area. By building the input datasets into a GIS and converting them to grids the EUZIT algorithms can be applied in GIS using the “map calculator” functions. Within the GIS it is also possible to carry out a sensitivity analysis to optimise the weightings (and ratings) per factor. Depending on the scale of the application and the degree of spatial variability, the possibility does exist, as found in the two case studies (see Chapter 6), that the initial spatial variability is “lost” due to the relatively broad ranges within the rating classes. One could refine the rating classes to enhance spatial variability in vulnerability. Further

work is recommended, however, on refining the ratings based on the scale of the study and data availability and on scientifically motivating the weightings.

GIS may also be coupled with *process-based* models that simulate physical processes in the environment. One such a model is UGIf which estimates recharge fluxes of organic pollutants (BTEX) in an urban environment. The model strictly deals with the unsaturated zone and was originally developed for selected areas of the unconfined Birmingham aquifer in the UK (Thomas et al., 2001; 2004; 2006). To make it suitable for South African conditions it was adapted to include various vulnerability assessment methods. An overview of the UGIf model is given in Section 5.2.

5.2 Overview of the UGIf model

UGIf is a process-based urban recharge pollutant flux model written in the Avenue programming language within ArcView GIS (version 3.2) and is primarily meant for the estimation of groundwater recharge pollutant fluxes of specific pollutants viz. BTEX (benzene, toluene, ethyl benzene and Xylene), nitrate and chloride to an urban unconfined, primary aquifer. The software packages required to run UGIf model are ArcView GIS 3.x version (ver 3.1 or 3.2 or 3.3) and its extension Spatial Analyst. UGIf accommodates the following processes (with their calculation method indicated in brackets):

- Infiltration, runoff and recharge (using the NRCS curve number method and water balance calculation based on estimates of evapotranspiration and soil moisture deficit for a given time)
- Interflow (also called lateral flow) of infiltrated water (empirical index approach);
- Volatilization of BTEX compounds in recharge water (Henry's law);
- Sorption of BTEX compounds (distribution coefficient); and
- Degradation of BTEX compounds (first order decay).

For modelling the above processes UGIf has various menus and submenus in its View document, such as:

- Direct Recharge
- Indirect Recharge
- BTEX NPS Pollution
- BTEX Petrol
- Groundwater Vulnerability Assessment

Figure 5.1 shows the interface of the UGIf model for the assessment of Non-Point Source (NPS) pollutant fluxes of BTEX.

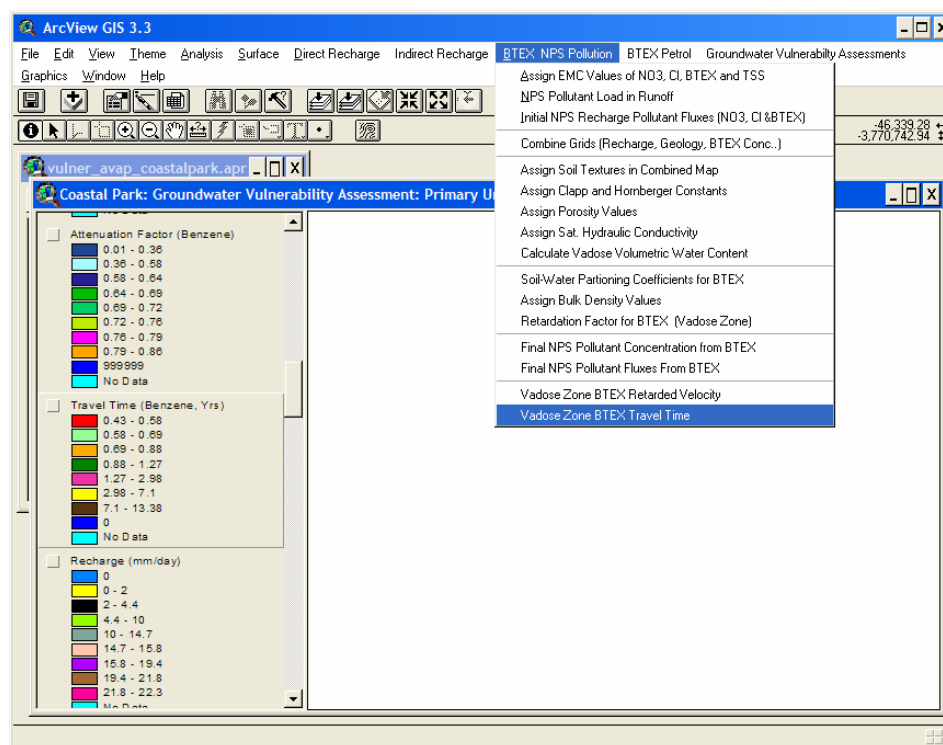


Figure 5.1: Interface of the UGIf model for assessing NPS BTEX pollutant fluxes.

5.2.1 Assessment of recharge and pollutant fluxes in UGIf

A simplified flow chart of estimating pollutant mass fluxes reaching the water table is given in Figure 5.2. A land use / land cover classification allows the production of a land cover map. To each land cover class attributes are assigned which relate to permeability, runoff and water quality. With meteorological data and the land cover related runoff characteristics, an estimate of ‘potential recharge’ for each of the land use classes can be made, where potential recharge is defined here as ‘actual recharge’ (i.e. water reaching the water table) plus interflow. An estimate of the potential mass flux (i.e. flux before interflow, evapotranspiration, and reaction) at the water table can also be made using runoff water quality data associated with the land cover classes. Interflow is estimated from geological maps and used to convert the potential recharge estimates into ‘actual recharge’.

The time taken to pass through the unsaturated zone can be estimated using the actual recharge estimates, hydraulic properties related to the geological units, (reversible) sorption properties related to each geological unit, and unsaturated zone thickness as calculated from land surface and water table maps. Using pollutant-related reaction properties and the estimates of time taken to pass through the unsaturated zone, the decay of degrading pollutants can be calculated, and hence the pollutant mass flux at the water table. Solute

concentrations in recharge waters, corrected for evapotranspiration where necessary, are also calculated.

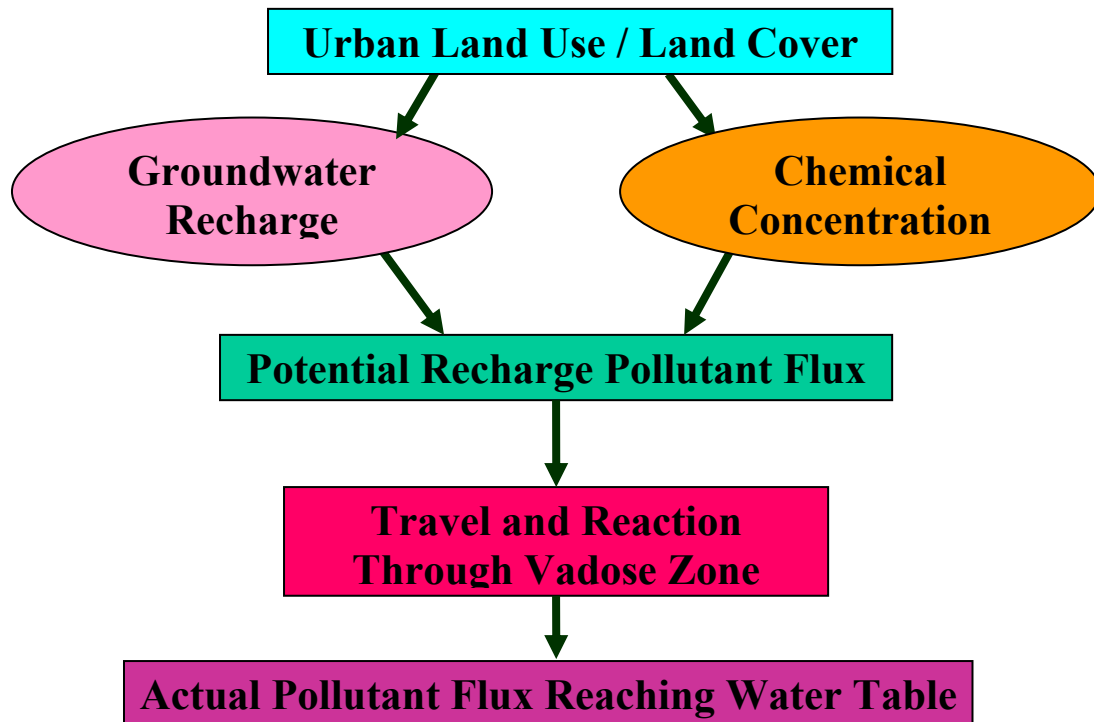


Figure 5.2: Simplified flow chart for estimating pollutant mass fluxes at the water table.

5.2.2 Direct recharge

The conceptual model for calculating direct recharge is shown in Figure 5.3. The term ‘initial loss’ signifies intercepted rainfall which ultimately does not infiltrate (vegetation and building interception / depression or detention storage). Formal definitions of infiltration, potential recharge, and actual recharge as used here are:

$$\begin{aligned}
 \text{Infiltration} &= \text{Rainfall} - \text{Initial Losses} - \text{Runoff}; \\
 \text{Potential Recharge} &= \text{Infiltration} - \text{Actual Evapotranspiration}; \text{ and} \\
 \text{Actual Recharge} &= \text{Potential Recharge} - \text{Interflow}
 \end{aligned}$$

where actual evapotranspiration is the evapotranspiration taking into account soil moisture availability.

Infiltration

Infiltration requires estimates of rainfall, initial losses, and runoff. Rainfall estimates are assumed to be available, but estimating runoff and initial losses is less straightforward. After considering various available methods for runoff estimation, the US-Natural Resources Conservation Service (NRCS) selected the Curve Number (CN) method as the appropriate

method. This empirical method is applicable in situations in which daily rainfall is available (US EPA, 1998a, b). It is simple, requires few input parameters, and has been widely applied in the field, including in urban catchments (US EPA, 1998a, b). However, it is accepted that the method, especially in the form applied here, is a considerable over-simplification of a complex set of processes, and further work will be necessary to justify its use and, when applied, parameter assignments. It will suffice in the present context as an example runoff-estimating formulation.

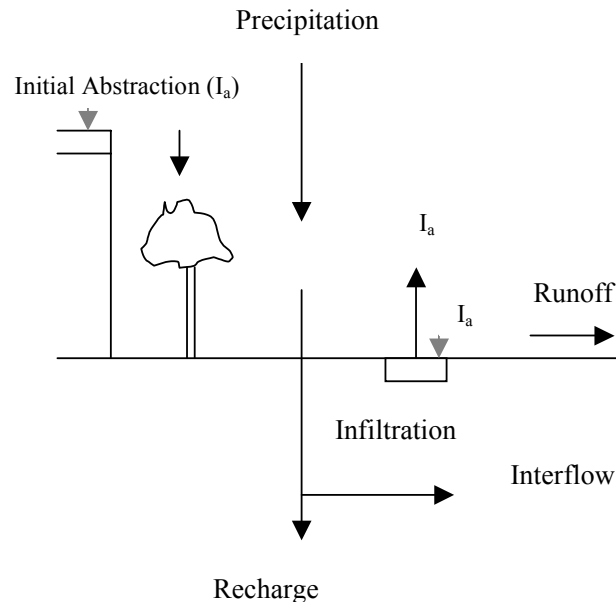


Figure 5.3: The conceptual model for the direct recharge calculations.

Potential recharge

For non-vegetated areas, the potential recharge is estimated with (post infiltration) evapotranspiration set to zero. It is assumed that once into the ground, the water is unlikely to be removed by evapotranspiration. This may not be true where roads are tree-lined. In vegetated areas, the calculation procedure takes into account the soil moisture deficit parameter and actual evapotranspiration.

Actual recharge

Actual recharge is calculated from potential recharge by subtracting interflow. Interflow depends largely on slope, porosity, storage capacity, the hydrologic soil group (HSG), average moisture content, effective permeability, permeability anisotropy, and lateral continuity of a perching horizon. Given the complexity of the process, rigorous calculation of interflow was not attempted. Instead, it was decided to develop a simple model based on indices reflecting what were viewed as the four most important parameters: slope, specific retention (soil storage capacity), permeability anisotropy ratio of the formation (K_h/K_v), and the presence or absence of low permeability deposits underlying the more permeable deposits at the surface. When calculating interflow in this model, a weighting factor is assigned by the

user to each of the four interflow indexes, so that the relative importance of each can be assigned.

5.2.3 *Non-Point Source (NPS) Pollution Flux Model*

Flux rates are calculated for non-reactive pollutants in surface water and for non-reactive and reactive pollutants at the water table.

Flux rates for non-reactive pollutants in surface runoff

Non-Point Source pollution represents the cumulative effects of all of the landuses and associated human activity in a catchment. Models that try to reflect each activity require large quantities of data, and these are rarely available. Thus, the most common method of approximating NPS pollution uses long-term average contaminant loadings for common land uses. This approach is based on the US National Urban Runoff Program (US EPA, 1983), and has been followed in many other countries. In this approach, Event Mean Concentrations (EMC) are defined for each landuse. These EMCs are assumed to be determined only by the landuse, and to remain constant independent of the duration and intensity of the rainfall events. EMC values are available in the literature (Lopes and Dionne, 1998; Delzer et al., 1996; Shepp, 1996). The EMC approach is worryingly simplistic, but until quantitative relationships between rainfall quantity and quality properties become available for urban areas, there is little point in making the model more sophisticated.

The input data for the calculation of pollutant flux rates in runoff are therefore: the landuse grid, the grid of average annual runoff volume calculated by the recharge model, and the associated EMC values for each landuse for each of the selected pollutants. An Avenue script was written linking the EMC value of various pollutants to the land use types. The EMC grid is then multiplied by the grid of average annual rainfall runoff. The result is the annual surface runoff loading for the NPS pollutant in each grid cell.

Flux rates for non-reactive pollutants at the water table

EMC values can also be used for estimating the NPS pollutant fluxes in the infiltrating water. The infiltrating water is subject to evaporative loss across the soil-air interface, and hence the concentration of the recharge water will be higher than that of the infiltrated water.

Flux rates for reactive pollutants at the water table

As they pass through the unsaturated zone, pollutants in the infiltrating recharge water may be subjected to various processes including sorption, volatilization, and biodegradation. In the current model, volatilization, linear sorption and first order decay is taken into account, but other formulations would also be possible. Pollutant fluxes are estimated through four stages, viz.:

1. Estimation of volumetric water content in the unsaturated zone;
2. Calculation of soil-water partitioning coefficients;
3. Calculation of retardation factors; and
4. Calculation of concentration and mass fluxes at the water table.

For further details on the above calculations, the reader is referred to Appendix 12 : “GIS-based algorithms for vulnerability assessment”.

5.3 Modified UGIf model

The UGIf model was revised to make it suitable for South African conditions and for groundwater vulnerability assessments using process based approaches. One modification included the editing of the script of land use grid map preparation in order to accommodate for different land use / land cover types which occur in South Africa. Currently this algorithm can write class names or descriptions of 45 types of possible land use units. A literature review on vulnerability assessment was carried out to find suitable screening level vulnerability assessment models which could be easily developed using ArcView GIS. Apart from the travel time model for BTEX compounds, three new screening level models for vulnerability assessment and a simple approach to assessing intrinsic vulnerability of conservative contaminants are incorporated in the model.

Screening level models are relatively simple, easy-to-use, require very little input data and provide a management decision support. Their major areas of application are: management of water resources (regional planning as related to groundwater control), formulation and implementation of regulatory policies (zoning, land use alterations and practices that protect groundwater quality), identification of “hot-spots” and selection of pollution abatement strategies, design and management of groundwater monitoring programs. The screening level models chosen for implementation in UGIf are:

- The Attenuation Factor model of Rao et al. (1985)
- The Leaching Potential Index Model of Meaks and Dean (1990) and
- The Ranking Index Model of Britt et al. (1992).

These models as well as the vulnerability of conservative contaminants are briefly discussed below.

5.3.1 The Attenuation Factor (AF) model

In order to facilitate the classification of pesticides according to their groundwater pollution potential, Rao et al (1985) developed the attenuation factor methodology that includes intrinsic properties of pesticides, hydrologic conditions and soil properties. Rao et al. (1985) formulated an Attenuation Factor (AF) index which denotes mass emission of a chemical from the unsaturated zone to groundwater as:

$$AF = \frac{M_2}{M_1} = \exp \left[\frac{-0.693 R_f Z \theta}{q T_{1/2}} \right]$$

where:

M_1 = initial mass of chemical applied at the ground surface;

M_2 = mass of chemical exiting the vadose zone;

$T_{1/2}$ = the half life period of the chemical; λ = first order degradation rate coefficient for the chemical;

R_f = Retardation factor;

Z = vadose zone depth;

q = net recharge rate obtained from a water balance calculation.

The retardation factor for volatile organic compound/pesticides can be calculated as:

$$R_f = 1 + (\rho_b K_d + (\theta_s - \theta) K_H) / \theta$$

where:

ρ_b = bulk density of the soil;

ε = air-filled porosity;

θ = the volumetric water content of the soil;

θ_s = the saturated water content of the soil on a volume basis;

K_d = the partition coefficient for the pollutant in the soil; and

$$K_d = K_{oc} f_{oc}$$

where K_{oc} is the organic carbon partition coefficient, f_{oc} is fraction of organic carbon content; K_H is the dimensionless value of Henry's law constant.

Here R_f includes the effects of soluble-vapor phase distribution, therefore this method is applicable to volatile organic compounds. For non-volatile organic compounds the normal retardation factor equation $R_f = 1 + (\rho_b K_d) / \theta$ can be used.

5.3.2 Leaching Potential Index (LPI) model

LPI is a methodology for ranking sites on the basis of their susceptibility to groundwater contamination. This method is a simplification of the one dimensional mass balance equation for the convective transport-dispersion-reaction process of solutes in a homogeneous porous medium. Assuming steady state conditions and negligible dispersion, Meeks and Dean (1990) simplified the mass balance equation to:

$$\frac{C_2}{C_1} = \frac{M_2}{M_1} = \exp \left[\frac{-0.693 R_f Z \theta}{q T_{1/2}} \right]$$

The leaching potential index LPI can be calculated as:

$$LPI = 1000 \left[\frac{\frac{q}{\theta}}{\left(\frac{0.693}{T_{1/2}} \right) R_f Z} \right]$$

where 1000 is a constant that converts the LPI into a practical range. The term within the parenthesis is an indication of the vulnerability of a site. High values indicate greater susceptibility to contamination.

5.3.3 Ranking Index (RI) model

The Ranking Index model is a methodology developed by Britt et al. (1992) for streamlining the pesticide registration and approval program of the Florida Department of Agricultural and Consumer Service in the USA. The ranking index (RI) for a chemical denotes the vulnerability to groundwater contamination by that compound. RI is expressed as:

$$RI = \left[\frac{0.693 R_f Z}{\left(\frac{q}{\theta} \right) T_{1/2}} \right]$$

This model requires the setting up of a threshold value for RI (e.g. 500); thus a chemical with an RI of 500 or higher for a particular site was considered for registration. If the RI is less than 500, then a complete analysis involving studies on leaching, adsorption/desorption, hydrolysis, soil dissipation, and groundwater monitoring was required for registration.

5.3.4 Vulnerability of conservative contaminants

Assessment of the intrinsic vulnerability of conservative contaminants can be carried out based on the evaluation of vertical travel time from the land surface to the aquifer. The travel time through the vadose zone can be calculated using the simple formula:

$$T_{\text{time}} = \frac{z \theta}{V_d}$$

where:

T_{time} = travel time (years);

z = vadose zone depth (m);

θ = average moisture content or volumetric water content; and

V_d = average recharge rate (m/day).

Witkowski and Kowalczyk (2004) carried out an assessment of groundwater vulnerability for conservative contaminants in Poland using a similar approach (one of their equations matches this approach).

All of these four vulnerability assessment models were programmed within ArcView GIS using the Avenue programming language. Two Avenue scripts were written; the first one implemented the three screening level models in one model run. The script has to be run separately for each compound of interest. The second Avenue script implemented the vulnerability assessment model for a conservative contaminant, for example, chloride.

5.4 Data requirements and outputs

The input data required for modeling direct recharge and non-point source (NPS) pollutant fluxes in runoff and recharge are:

- Meteorological data (rainfall, evapotranspiration and soil moisture deficits);
- Land use/ land cover map;
- Soil map or Hydrologic soil group map;
- Geological map with hydraulic and geochemical attributes;
- Event mean concentration (EMC) values for each land use type/class; and
- Topographic and water table depth data in grid form.

The hydraulic and geochemical attributes needed are: porosity, bulk density, specific retention, presence of clay (clay index), horizontal and vertical hydraulic conductivity values,

fraction of organic carbon content, half lives of BTEX compounds etc. Standard model outputs include the following:

- Distribution of surface runoff;
- Cumulative infiltration;
- Potential recharge;
- Ground level slope;
- Interflow;
- Actual recharge;
- Pollutant fluxes in surface runoff;
- Travel times of each pollutant through the unsaturated zone; and
- Pollutant fluxes and concentrations at the water table.

For vulnerability assessments using the three screening level algorithms of UGIf, it requires a combined grid containing attributes of average recharge rate (m/day), soil moisture or volumetric water content, vadose zone depths (m), and the retardation factor values. The input required for vulnerability assessment for a conservative contaminant is a combined grid containing attributes of average recharge rate (m/day), soil moisture or volumetric water content and vadose zone depths (m).

5.5 Software application

UGIf currently estimates groundwater vulnerability of a primary unconfined aquifer (from NPS BTEX pollution). For groundwater vulnerability assessment of primary unconfined aquifer from non-point source BTEX pollution, the user has to open the project file `ugif_vulnerabilty.apr`, input various data and run each program (submenus) in three main menus (viz. Direct Recharge, BTEX NPS Pollution and Groundwater Vulnerability Assessment). The following steps are involved in vulnerability assessment for BTEX compounds using the UGIf model:

1. Creation of input data folder (for example, `C:\vulnerability`) and copying of ArcView 3.x compatible format input data;
2. Creation of a working directory or folder (e.g., `C:\vulnerability\work`) for storing subsequent GIS files created while running the model;
3. Opening of the ArcView GIS project file (e.g., `ugif_vulnerabilty.apr`);
4. Estimation of direct recharge (output in grid format);
5. Assessment of Non Point Source Pollution in Recharge (initial concentration);
6. Preparation of vadose zone depth map (grid format);

7. Preparation of geology grid map;
8. Combining grids of recharge, BTEX concentration, geology and vadose zone depth;
9. Assigning of soil textures, and Hornberger constants, porosity, saturated hydraulic conductivity and calculation of vadose zone volumetric water content using the Clap and Hornberger method (Clap and Hornberge , 1978);
10. Calculation of soil-water partitioning coefficient values for BTEX;
11. Assigning of bulk density and calculation of vadose zone retardation factors;
12. Assessment of final concentrations and fluxes of NPS pollution;
13. Running of three programs of vulnerability assessments such as:
 - a. Calculation of vadose zone travel time of BTEX compounds (running of last program called 'Vadose Zone BTEX Travel Time' under the menu 'BTEX NPS Pollution');
 - b. Running of the program for the assessment of groundwater vulnerability for conservative pollutants (first program under menu 'Groundwater Vulnerability Assessment');
 - c. Running of the program for the assessment of groundwater vulnerability for BTEX compounds (second program under menu 'Groundwater Vulnerability Assessment').

From the above steps it is clear that the user has to come up with a series of inputs and spatial data for running this model. Before running the project file of the model, the user has to be ready with a set of spatial inputs. On opening the project file, a start up script will initiate by which the user will be asked to specify a data folder, a working folder and select input maps of land use and hydrologic soil group. After adding these two data layers the user can select the menu of Direct Recharge and run various programs in this menu which assists in estimating recharge. After assessing direct recharge one can go for the other programs in the model (such as the menus of 'BTEX NPS Pollution' and 'Groundwater Vulnerability Assessment').

Combining grids of recharge, BTEX concentration, geology and vadose zone depth (step 8) is done using the submenu 'Combine Grids' under BTEX NPS Pollution menu. Before running this program the user has to first add these themes into a View and while running this program the user will be asked to select appropriate grid and its attribute field for combining. Steps 9, 10 and 11 are straightforward using the respective submenus under BTEX NPS Pollution menu.

The reader is referred to Appendix 14  on "Guidelines for developing and compiling vulnerability maps using GIS" for detailed instructions on how to operate the modified UGIf model.

5.6 Limitations of UGIf and reliability of prediction

The model takes into account the principal processes involved, and, as it is incorporated in a GIS, it allows spatial heterogeneity in parameter values to be investigated. A major limitation of the UGIf model is the way in which time is being dealt with. It is assumed that land use and land use-related properties do not vary within the 'time-slice' or period being considered by the model. Within the modelling period, steady-state conditions are assumed for the movement of water and solutes through the unsaturated zone. Thus, individual recharge pulses are not tracked: residence time in the unsaturated zone is calculated on the basis of the averaged recharge rate, but it is only used, with a delay arising from any sorption, to estimate degradation/decay of the pollutant concentration. Without incurring considerable computation times, it would be difficult to track individual recharge pulses.

The different sub-models in UGIf make use of many input parameters (both spatial and non-spatial data) and the accuracy of their predictions is dependent on the assumptions made in each of the sub-models and the accuracy of the input data used. Testing the UGIf model for another particular region in South Africa requires a variety of spatial and non-spatial inputs. Scarcity of input data (e.g. land use information, evapotranspiration and soil moisture deficit data, hydraulic properties and geochemical parameters like fraction of organic carbon, etc.) limits validation the model.

Environmental models are simplified representations of real systems, and uncertainty is always associated with their representations. In many cases the systems, especially urban groundwater systems, are heterogeneous, where a wide range of parameters with a wide range of possible values for them control the complex behaviour of the system. In the case of recharge and solute transport simulations of urban environments, the hydraulic and transport parameters are generally not known in sufficient detail. Most of the input parameters in the present GIS based urban pollutant flux models are derived from literature values and therefore predictive runs and the results obtained from them are subject to much uncertainty in relation to the complex heterogeneity of the urban system being modelled. There may also be additional uncertainty relating to whether the conceptual model with simplified analytical equations is fully applicable to the field situation in an urban area (Thomas, 2001).

Results from the modified UGIf, however, can be compared with other (independent) methods. The EUZIT Spreadsheet tool for example (Chapter 3) provides an averaged vulnerability of a particular site and can be compared with the spatial vulnerability assessment by the UGIf model, especially with regards to the LPI and the travel time of conservative and non-conservative organic contaminants.

5.7 References

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CHAPTER 6: **CASE STUDIES**

Two study sites were selected to illustrate the use of AVAP's approaches to the assessment of aquifer vulnerability to contamination in an urban catchment:

- The Goedehoop irrigation site near Secunda, and
- The Coastal Park waste disposal site near Cape Town.

6.1 Goedehoop study site - Secunda

Sasol has operated a large petrochemical facility at Secunda (Mpumalanga) for over two decades. Surplus ammonia rich process effluent containing elevated concentrations of fluoride and boron have been disposed of by irrigation, exploiting evaporation to get rid of the excess water. Effluent has been irrigated onto land from 1991 to 2000 at the Goedehoop site (Figures



Figure 6.1: The Goedehoop irrigation site with the Sasol Synfuels complex in the background.

6.1 and 6.2). Sasol has monitored soil properties and groundwater quality (Loxton Venn & Associates, 1991; Ginster, 1993 and 1994; Jasper Muller Associates, 1999; Sasol, 2002; and Vermeulen, 2004) and indications are that groundwater contamination occurs in the vicinity of the effluent irrigation facilities.

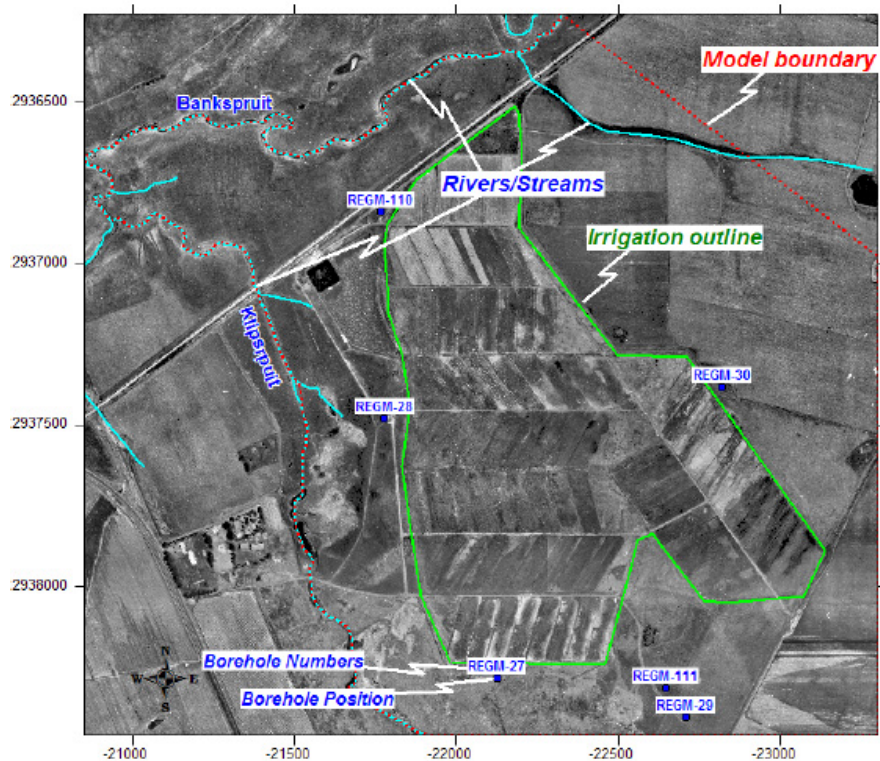


Figure 6.2: The Goedeheop irrigation site, showing streams and monitoring borehole locations.

6.1.1 Conceptual model of the Goedeheop study site

The climate is sub-humid, with mean annual rainfall of 700 mm, and Class-A pan evaporation amounts to 1700 mm per annum. The site is underlain by an unconfined to semi-confined weathered/fractured aquifer in Karoo sediments. Two major soil types occur; a duplex Swartland form (sandy A horizon over a clay-rich B-horizon) upslope, and a Rensburg form (black smectitic clay) in the low-lying areas. The geology and the duplex soil association are both representative of large parts of the South African interior, especially the Highveld.

The groundwater levels measured at the five monitoring boreholes (Figure 6.2) range from 3 to 16 m. Figure 6.3 presents a schematic cross-section through the Goedeheop study site. There are three prominent geohydrological layers in the area:

- Layer 1: Topmost layer of shallow weathered zone aquifer, consisting of soil and underlying completely weathered rock, varying between 5 and 13 m in depth. It is believed to be the most hydro-geochemically active layer.
- Layer 2: Bottom layer of shallow weathered zone aquifer, consisting of highly weathered to weathered hard rock, 20 – 30 m in depth. It underlies Layer 1. Although retardation is likely through sorption of metals, it is hydro-geochemically very inactive compared to soils.

- Layer 3: Hard rock of relatively low permeability.

Groundwater level measurements indicate a heterogeneous, fractured environment, where layers 1 and 2 may be dewatered locally. There are two flow components of significance (which depend on the hydraulic pressure head distribution):

- Vertical flow: from surface into Layer 1, and through Layer 1 to Layer 2.
- Horizontal flow: within Layer 1 and within Layer 2.

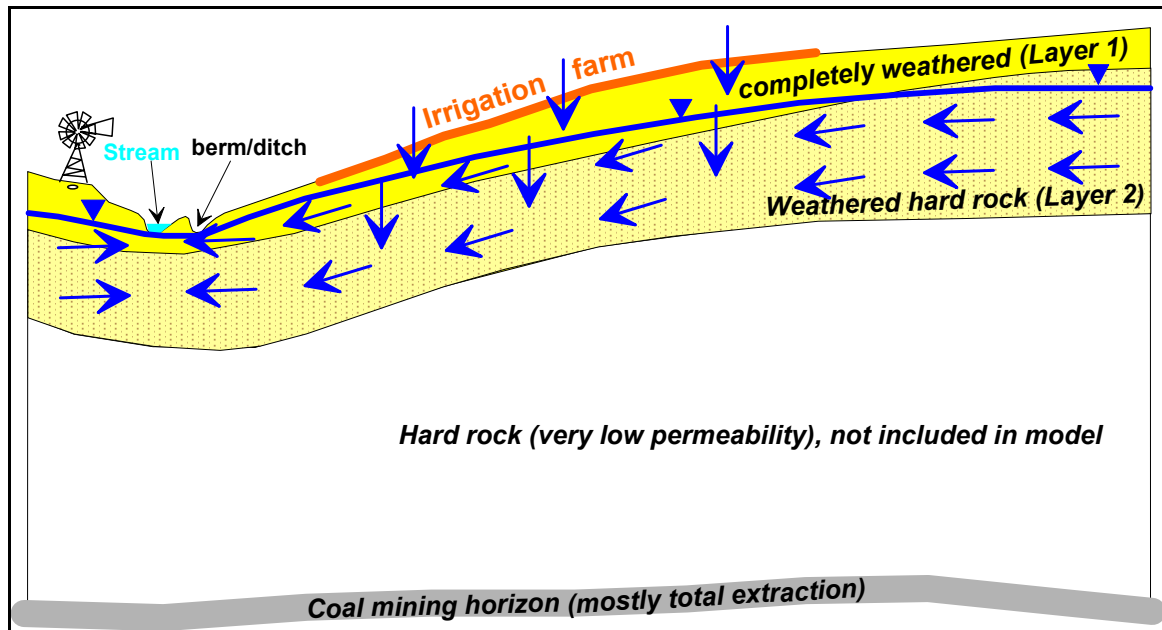


Figure 6.3: Schematic cross-section through the Goedehoop study site.

Saturated hydraulic conductivity (K_{sat}) values for the Goedehoop site were estimated to be between 0.05 and 0.1 m/day (JMA, 1999). The clayey soils swell when in contact with water. The swelling and shrinking of the clays will also inevitably lead to the formation of cracks. It is thus safe to assume that preferential flow will occur to at least some depth.

6.1.2 Unsaturated zone vulnerability

From historical data it is evident that there was already in the early 1990s a build-up of contaminants, especially anionic solutes (B, F, Cl, NO_3 , SO_4), in the upper part of soil profiles but that following the cessation of much of the irrigation activity in 2000 the concentration of contaminants at shallow depth decreased. Sampling in 2002 at Indaba (near Goedehoop) revealed that solute migration had taken place into deeper soil layers (Figure 6.4).

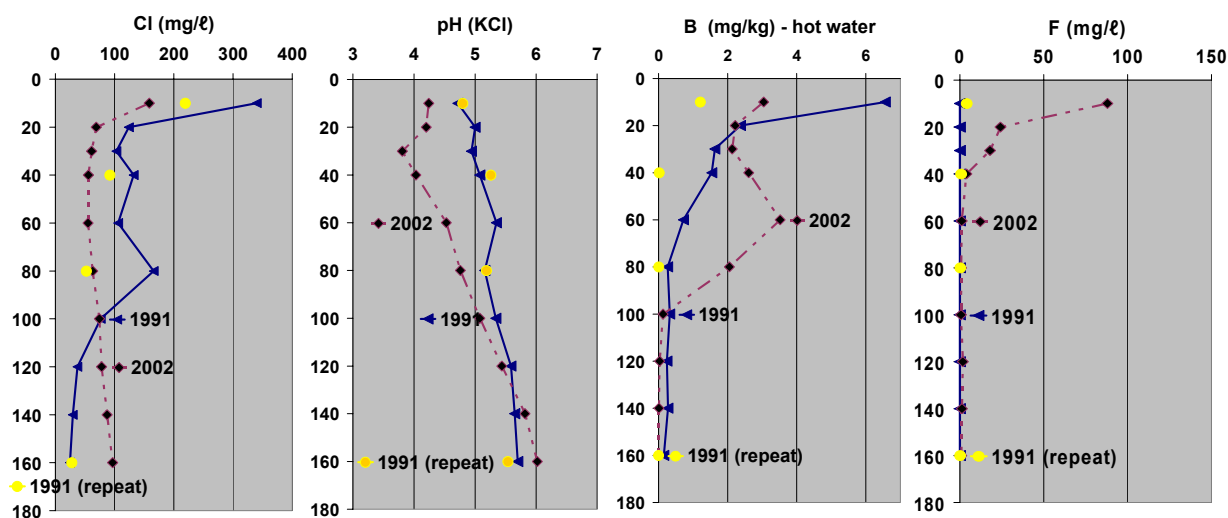


Figure 6.4: Illustrative Chemical profiles for Cl, pH, B and F plotted for samples taken in 1991 and 2002 from a site at Indaba adjacent to Goedhoop (Ginster, 2004).

Vulnerability of the soil zone

Soils information was collected during 2006, allowing for a specific vulnerability classification to be related to concentrations of contaminants (chiefly F and B) in the soil profile. About 60 soil samples were collected by augering 12 soil profiles at 20 cm depth intervals to a depth of 1 m in the area and analysed for pH, EC, CEC and composition, Al, Fe, organic C, B and F (see Appendix 19). Vulnerability ratings were calculated for leaching of three classes of contaminants: metal, anionic and non-polar organic contaminants. These ratings were calculated first for individual soil horizons and then for each soil profile. The vulnerability ratings integrate the chemical, hydraulic and climatic indices (Appendix 19). In Table 6.1, vulnerability ratings for each of the 12 soil profiles are shown in relation to soil form and family classification and to the location of the profiles. These profile-based vulnerabilities were plotted against the mean profile values of S (CEC) for cationic contaminants (Figure 6.5) and C(arbon) content for anionic and organic contaminants to illustrate how links between vulnerability ratings and sorption-related variables may be preserved even after performing a depth-weighted calculation for the profile as a whole and after taking into account physical attenuation characteristics related to soil water balance. The integrated chemical vulnerability of the soil zones formed part of the input of the EUZIT spreadsheet Tool for determining an averaged unsaturated zone vulnerability to contamination.

Table 6.1: Calculated vulnerability ratings for 12 soil profiles at Goedehoop in relation to profile location and soil classification.

Field Location	Soil family	Integrated Vulnerability Score to contamination		
		Cationic	Anionic	Organic
EJ0057	Rg2000	5.2	6.0	6.5
EJ0092	Rg2000	0.5	1.5	1.1
EJ0082	Rg2006	0.6	2.0	1.6
EJ0084	Rg2006	1.7	6.0	5.7
EJ0075	Rg1000	1.7	5.7	5.7
EJ0062	Rg2000	2.3	3.9	5.7
EJ0038	Rg2000	4.4	6.2	7.1
EJ0029	Va1122	3.6	5.7	5.7
EJ0019	Va1122	3.0	5.7	6.0
EJ0041	Va1122	3.0	5.7	5.7
EJ0054	Va1121	3.4	5.2	5.7
EJ0032	Va1121	3.8	6.0	5.7

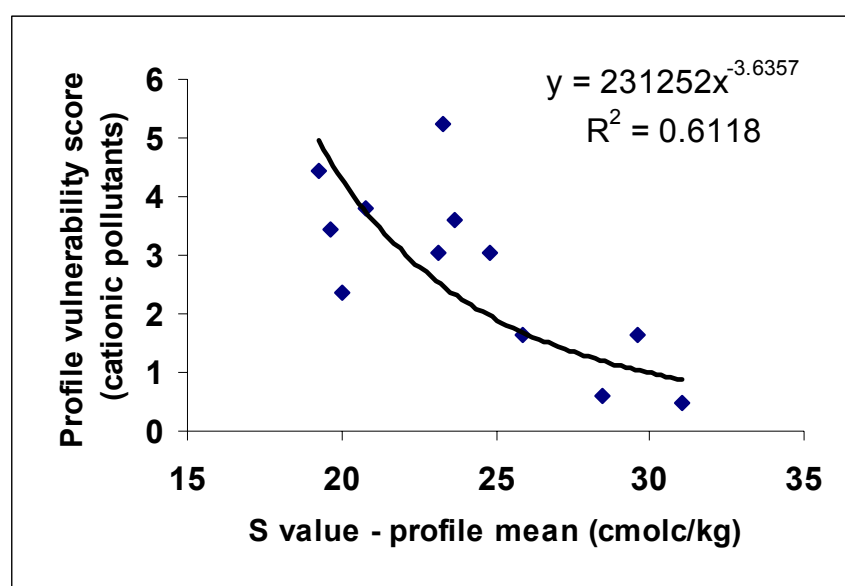


Figure 6.5: Profile vulnerability ratings for metal contaminants in relation to the S (=CEC) value.

EUZIT application

Given the information collected for the Secunda site, an assessment of groundwater vulnerability was carried out with the Excel-based Unsaturated Zone Index Tool (EUZIT). The results are summarized in Table 6.2 and rank the groundwater vulnerability of the Secunda site as medium (score 4.4). In the example of a persistent chemical like 1,1,1-Trichloroethane, the groundwater vulnerability is ranked as medium-high (score 5).

Table 6.2: Vulnerability assessment of the Secunda site using unsaturated zone information (Appendix 20 ).

Factors	Description	Comments	Score
Thickness of the unsaturated zone	5.4 – 15.1 m (average 6.65 m)		(1X3)=3
Hydraulic properties	1. Sandy clay, silty clays 2. $K_{sat} = 0.003 \text{ m d}^{-1}$ 3. $K_{sat} = 0.072 \text{ m d}^{-1}$ (van Genuchten-Mualem model for sandy clay)	1. Sieving analysis - modelling 2. Literature	(1X3)=3
Flow mechanism	Matrix and Preferential	Surface cracks, swelling clays	(3X3)=9
Slope	1.5%	Bare soil and grass	(2X1)=2
Recharge	1. Qualified guess = 19 mm a^{-1} 2. No irrigation = 21 mm a^{-1} 3. During irrigation = 24.5 mm a^{-1}	Irrigation increases recharge (artificial recharge)	(3X2)=6
Travel time	1. Thickness = 6.65 m 2. Effective porosity 20-25% 3. $K_{sat} = 0.003 \text{ m d}^{-1}$	Foster and Hirata (1995) equation: Gross surcharge: $> 1 \text{ a}$ Natural infiltration: $>> 1 \text{ a}$	(2X2)=4
Sorption capacity	1. Clays 2. Organic carbon content: 0.12–3.69%		(2X2)=4
Half-life	Contaminant specific	Long travel time, low conductance, medium sorption	(3X3)=9
TOTAL: Excluding Contaminant half-life			4.4 Medium
TOTAL: Including Contaminant half-life (1,1,1-Trichloroethane)			5 Medium-High

The EUZIT spreadsheet model was also used as the basis for carrying out a GIS-based vulnerability assessment of the Goedehoop site. The results of the previous work, mainly in the form of spreadsheet files and dxf modelling files, and input to other basic layers as required by the EUZIT model were compiled and georeferenced into a comprehensive GIS. The raster data layers had a 50 m cell size, which was considered an appropriate size to reflect the spatial variability that occurs on the site. The main spatial variability was found in the depth of the unsaturated zone, with values ranging from 5.3 to 15.2 m. According to the data sets available, there was little variation found in the geology and rainfall across the site.

For all 8 of the GIS layers, once they were rated they received a single value for the entire grid. The rating and weighting process resulted in a final GIS layer of “medium vulnerability” yet all spatial variability of the site was “lost”. With the refinement of the EUZIT ratings and weightings a relative vulnerability assessment map can be produced.

UGIf model application

The UGIf application was used to calculate direct recharge, non-point source pollution and vulnerability indices for the Goedehoop study site. For the calculations it was assumed that there is no recharge from natural water bodies (streams, vleis, wetlands and lakes). Areas of higher recharge are more likely to introducing contaminants to the aquifer. Thus the recharge distribution itself is an indication of vulnerability. Recharge rates underneath barren land, open ground and grassland are higher than in buildup areas. The recharge used in the model represents potential recharge after accommodating for an evapotranspiration of 4.65 mm/day.

The following vulnerability indices have been calculated for conservative contaminants (Chloride) and for dissolved organic contaminants (Benzene with an initial concentration of 4 microgram/l):

- Travel time for conservative and reactive contaminants
- Attenuation factor (AF)
- Leaching Potential Index (LPI), and
- Ranking Index (RI)

Figure 6.6 shows the calculated travel times for a non-reactive solute. The predicted travel times are classified using a 'quantile' classification. The travel times are up to 2.25 years. When compared with the results of reactive contaminant (benzene) travel times (up to 23.67 years) it is clear that non-reactive solutes reach the aquifer much faster than the reactive organic compound, which is subject to sorption, volatilisation and decay. The figure shows that the north-eastern and south-western sides have higher vulnerability. This is largely due to the small unsaturated zone thickness. The predicted vulnerability values from the travel time model or the screening models underneath natural water bodies differ from other landcover types - having either maximum values because of immediate entry or values of zero or infinite numbers which depends on the equation used in the model. As a result areas of natural water bodies are shown as -999 in the maps, for situations having zero values or an infinite number, and are highlighted in yellow (using a selection in ArcView GIS 3.2).

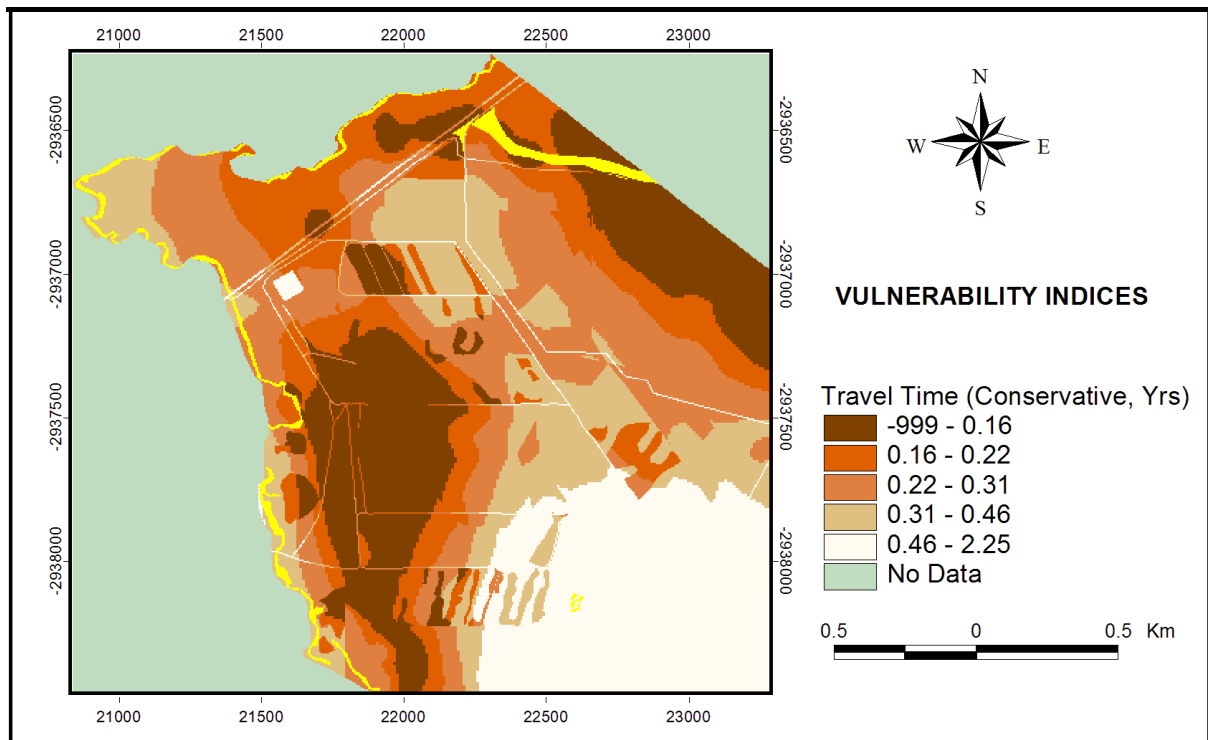


Figure 6.6: Distribution of travel time in years for a conservative contaminant, with shorter travel times (darker colours) indicating higher vulnerability.

Figure 6.7 shows the distribution of calculated leaching potential index (LPI) values. The index ranges from zero to 55815, with the higher values in areas with shallow unsaturated zone depths. The figure reveals which areas are vulnerable to benzene if a spill happens or if one applies uniform benzene contamination over the whole study area. The pattern of relatively high vulnerability in the north-eastern and south-western parts of the area closely resembles the patterns of vulnerability based on the travel time (Figure 6.6), attenuation factor and ranking index calculations.

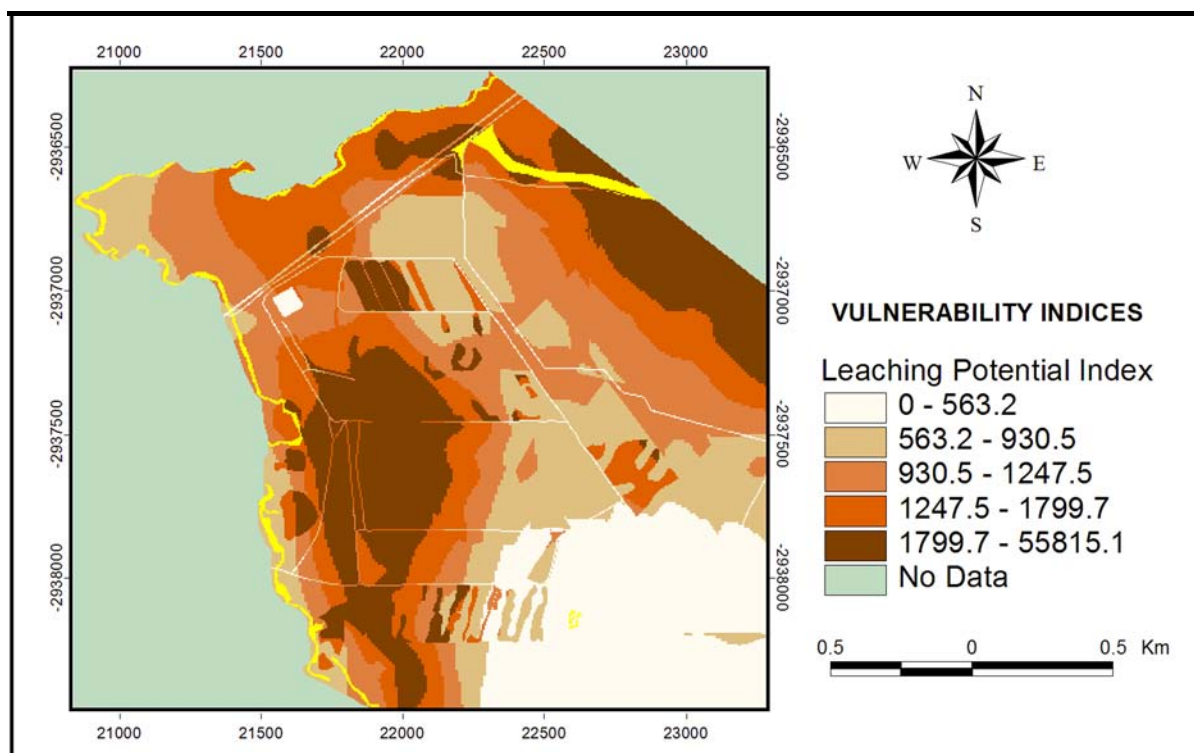


Figure 6.7: Leaching potential index values for Benzene in recharge water, where higher values (darker colours) indicate higher vulnerability.

6.1.3 Saturated zone vulnerability

Vulnerability of the saturated zone was evaluated for both inorganic and organic contaminants, assuming that the contaminants have bypassed the unsaturated zone. Simulation of contaminant migration in the aquifer was carried out by linking groundwater flow with geochemical processes; i.e. MODFLOW and the MT3D-MS code linked with PHREEQC-2 for inorganic contaminants and PHT3D, BIOPLUME III, the LNAPL Guide and BIOCHLOR for dissolved organic contaminants. The spatial impact of contamination was determined after 30 years of continuous irrigation, whereas the persistence of contamination was determined by ceasing irrigation after 10 years followed by 20 years of rainfall. The results for the Goedehoop site are presented in Table 6.3.

Regarding the saturated zone, using preset water quality thresholds, the spatial impact of the inorganic and organic compounds ranged between 120 and 380 m from the source and all the compounds are likely to persist in the aquifer for more than 30 years if irrigation at the Goedehoop site was only to take place for 10 years.

Table 6.3: Saturated zone vulnerability assessment results (after Appendixes 10 and 18 ).

Contaminant of Concern		Dual porosity sedimentary rock aquifer		
Source Type	Contaminant	Major physio-chemical controls	Spatial Impact (m)	Persistence after source removal* (yr)
Industrial Effluent Inorganic	Ammonium	Advection, dispersion and recharge	150	>300
	Fluoride		380	>300
Industrial Effluent Organic	Benzene	Retardation (foc + Kow), volatilisation, biodegradation	350	80
	Ethylbenzene		220	>100
	Toluene		165	>100
	Xylenes		150	>100
	PCE		120	50 (Anaerobic)
	TCE		350	100 (Anaerobic)

* These values are very site specific and depend on the initial concentrations, site conditions and point of measurement

6.1.4 Discussion

This case study demonstrated how the soil classification can be applied to derive vulnerability ratings for the soil zone. Future refinements of the classification are envisaged especially in relation to the hydraulic attenuation classes based on soil texture and the aridity index. Further work could also usefully be done on the soils collected at Secunda by combining them in leaching columns to represent reconstituted soil profiles which could then be tested for breakthrough behaviour with various categories of contaminants. Breakthrough behaviour could then be related to the vulnerability classes predicted by routine soil analyses.

The vulnerability of the unsaturated zone to contamination as derived from both the EUZIT spreadsheet program (incorporating the chemical vulnerability of the soil zone) and the UGIf model ranges from medium to high. This means that contaminants generated at the surface are likely to reach the water table and pollute the aquifer. This may have been expected due to the unconfined nature of the aquifer and the relatively shallow depth of the water table.

The spatial impact of the inorganic and organic compounds for the saturated zone ranged between 120 and 380 m from the source and all the compounds are likely to persist in the aquifer for more than 30 years following cessation of irrigation after 10 years.

The foregoing provides a basis for deciding on set back distances in relation to water abstraction points in the area.

6.2 Coastal Park waste disposal site - Cape Town

The Coastal Park waste disposal site serves the City of Cape Town and is located on the Cape Flats Aquifer (CFA). The impact of the Coastal Park waste disposal site (Figure 6.8) on the aquifer has been extensively studied by the Cape Town local authority and a variety of consulting firms and researchers (e.g. Ransome & Wit, 1992; Blight & Ball, 1995; and Novella et al., 1999). Numerous groundwater monitoring wells and mini-piezometers (positions shown in Figure 6.9) have been installed, including lines of wells to monitor down-gradient groundwater quality at various distances from the waste site.



Figure 6.8: The Coastal Park waste disposal site

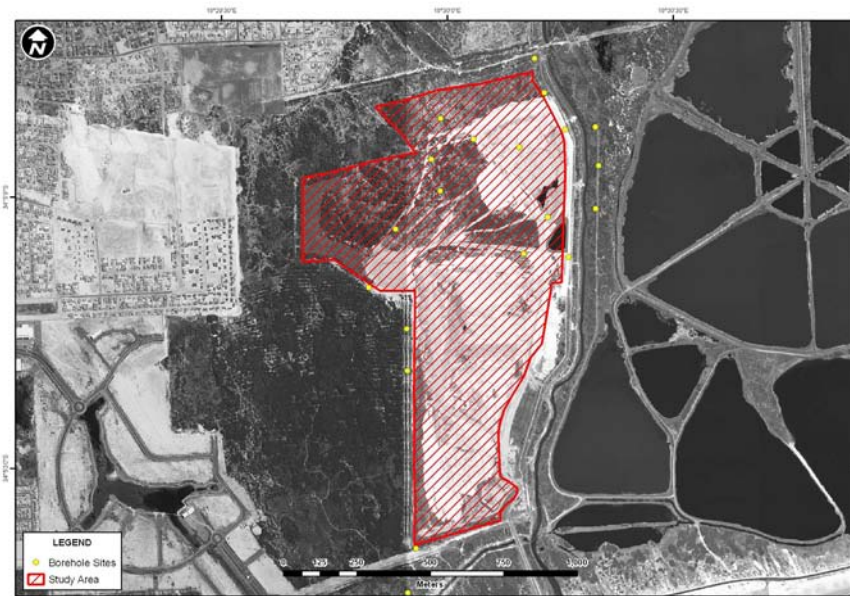


Figure 6.9: The Coastal Park waste disposal site and monitoring boreholes.

6.2.1 Conceptual model of the Coastal Park waste disposal site

The Cape Flats aquifer is primary and unconfined. It comprises a Quaternary sand succession (clean sands) which is similar to aquifers in other coastal areas such as the Swartkops aquifer in Port Elizabeth, and the Zululand coastal aquifer of Richards Bay. The lower part of the aquifer is bounded by a clay aquitard and the water table is in the range of 1 to 5 metres below surface. Regional groundwater flow in the CFA is to the west to Table Bay or to the south to False Bay. Major contaminants produced at the Coastal Park site are: nutrients (N, P, K), salinity, pathogenic micro-organisms, organic contaminants (fuels, solvents) and trace metals. Geochemical processes, low hydraulic gradients and rapid and abundant recharge of the aquifer may reduce its vulnerability to contamination to some degree – or at least enhance its capacity to recover from contamination.

6.2.2 Unsaturated zone vulnerability

EUZIT application

Table 6.4 summarizes the results of applying the EUZIT approach to vulnerability assessment at the Coastal Park waste disposal site, based on aquifer properties obtained at the UWC experimental research site. The unsaturated zone scores low in its capacity to attenuate contaminants and has a medium to high vulnerability class/rating (score 6.7). In the example of a persistent chemical like 1,1,1-Trichloroethane, the groundwater vulnerability index score was 7. The CFA is thus generally vulnerable to most types of contamination (Appendixes 9 and 17 .

Table 6.4: Vulnerability assessment of CFA using the Excel based unsaturated Zone Index Tool (Appendixes 9 and 17 ).

Factors	Description	Comments	Score
Thickness of the unsaturated zone	1-5 m (average 3m)	Some areas have water table at surface	(3X3)=9
Hydraulic properties	1. Sand, minor silt, clay lenses, heterogeneous 2. $K_{sat} = 15-50 \text{ m d}^{-1}$, $T = 30-980 \text{ m}^2/\text{d}$ 3. $K_{sat} = 16 \text{ m d}^{-1}$ (van Genuchten-Mualem model 100% sand). 4. $K_{sat} = 6 \text{ m d}^{-1}$ (van Genuchten-Mualem model 94% sand, 5% silt, 1% clay) 5. Literature $K = 15-91 \text{ m d}^{-1}$	1. Sieving analysis (UWC) 2. Repellency	(2X2)=4
Flow mechanism	Piston and Preferential	Macropore flow (burrows), funnel	(2X2)=4
Slope	0%	Bare soil and grass	(3X3)=9
Recharge	1. 10-13% of mean annual precipitation (Bredenkamp et al., 1995). 2. CMB = 10% of mean annual precipitation 3. $60-80 \text{ mm a}^{-1}$	1. Tritium profiling and CMB (Atlantis) 2. CMB (UWC CAT Site)	(3X3)=9
Travel time	1. Thickness = 3 m 2. Effective porosity = 25-40% 3. $K_{sat} = 15-50 \text{ m d}^{-1}$	Foster and Hirata (1995) equation: Gross surcharge: $< 1 \text{ h}$ Natural infiltration: $< 1 \text{ a}$	(3X2)=6
Sorption capacity	1. High silica, Ca sands. 2. The fraction of organic carbon of the sands (0.3-0.4%) is relatively low and sorption will thus be low (Sililo, 1997)	Peat layers can increase sorption capacity. Organic layers have been reported.	(3X2)=6
Half-life	Contaminant specific	High travel time, low sorption, thin unsaturated zone	(3X3)=9
TOTAL: Excluding Contaminant half-life			6.7 Medium-High
TOTAL: Including Contaminant half-life (1,1,1-Trichloroethane)			7 Medium-High

The EUZIT spreadsheet model was also used as the basis for carrying out a GIS-based vulnerability assessment of the Coastal park Waste disposal site. Again, with the re-classing of the grids all spatial variability was reduced to the single class, i.e. “High vulnerability”.

UGIf model application

The UGIf model and its newly developed vulnerability algorithms were applied to the Coastal Park data. The simulation of groundwater vulnerability assessment for the study area was performed using a groundwater recharge map generated for 30 mm rainfall. The calculation of groundwater recharge revealed again that areas underneath open

ground/grasslands receive higher recharge, whereas the aquifer under high density residential areas receives less recharge. The areas under roads and the effluent ponds (lined, with a low leakage rate) receive less recharge.

Figure 6.10 shows groundwater vulnerability indices for a non-reactive solute. The unsaturated zone travel time ranges from zero to 0.97 years only, which is much lower than the results for Benzene, which ranges from zero to 13.38 years. Clearly, non-reactive solutes such as chloride can reach the aquifer much faster than reactive organic compounds (such as benzene) which are subject to sorption, volatilisation and decay.

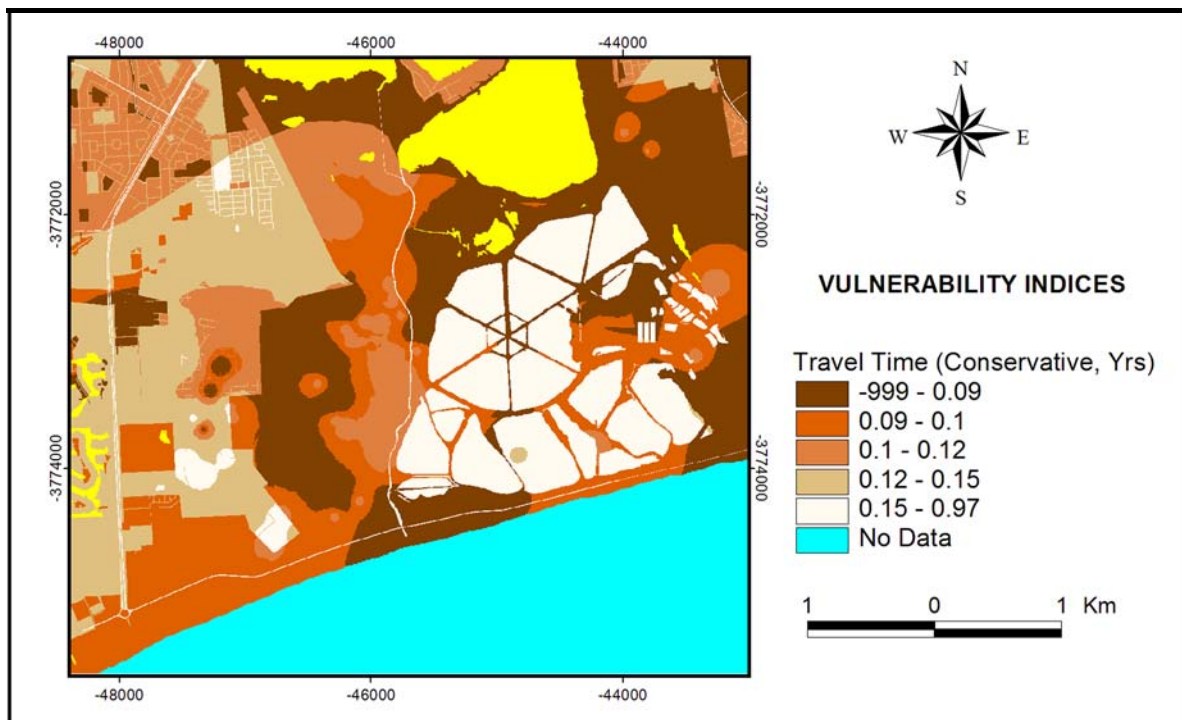


Figure 6.10: Distribution of travel time in years for a conservative contaminant at Coastal Park, with shorter travel times (darker colours) indicating higher vulnerability.

Figure 6.11 shows the vulnerability indices predicted for benzene from the leaching potential index calculations. It reveals which areas are vulnerable to benzene if a spill occurs or if one applies uniform benzene contamination over the whole study area. The leaching potential index values range from zero to 6545. From this map (and those for the attenuation factor and the ranking index) one sees a similarity in the distribution of vulnerability indices with the results obtained from the travel time calculations (Figure 6.10).

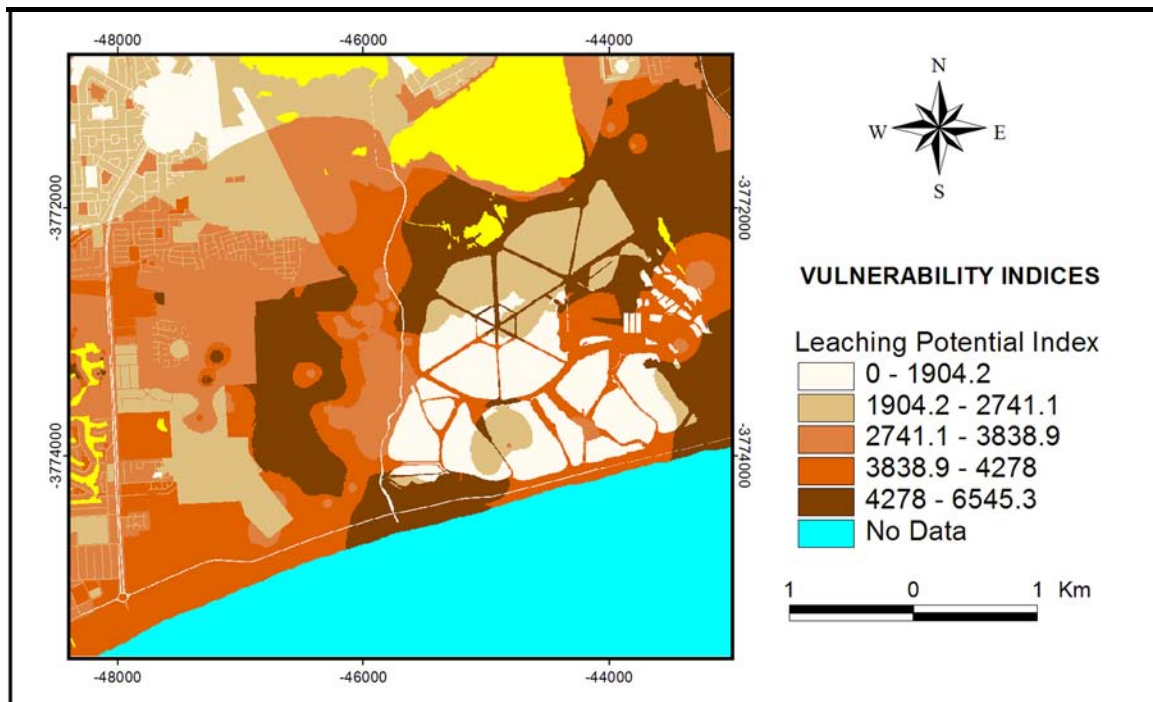


Figure 6.11: Leaching index potential values for Benzene in recharge water at Coastal Park, where higher values (darker colours) indicate higher vulnerability.

The pools around the sewage treatment plant have lower values, indicating lower vulnerability values, largely due to lower recharge. The open ground/grass land areas have higher vulnerability values, because of higher recharge. In all the maps residential areas have medium vulnerability, which corresponds to the medium recharge rates in these areas. Preliminary results thus suggest that for all five predictions there is a consistent pattern of vulnerability of groundwater to pollution at the Coastal Park landfill site. Based on the distribution of predicted vulnerability indices, one can say that in general the Coastal Park area is highly vulnerable to groundwater contamination.

6.2.3 Saturated zone vulnerability

For three types of contaminant sources: industrial effluents, domestic landfill leachate and acid mine drainage, the saturated zone vulnerability was evaluated for a hypothetical primary aquifer (coastal primary aquifer) using PHREEQC-2 and compared with a dual porosity aquifer developed in the weathered zone overlying sedimentary or igneous rocks (see also Section 4.2.2). Modelling of the saturated zone vulnerability revealed that the spatial impact following contamination by a landfill leachate and industrial effluent is larger and the persistence lower compared with the dual porosity aquifer, whereas for acid mine drainage it is the other way around (Appendix 10).

6.2.4 Discussion

The vulnerability of the unsaturated zone to contamination as derived from both the EUZIT spreadsheet program and the UGIf model is medium to high. This means that contaminants generated at the surface are likely to reach the water table and pollute the aquifer. This may have been expected due to the unconfined nature of the aquifer and the relatively shallow depth of the water table. Other important contributions to the unsaturated zone vulnerability at this site are recharge (relatively high), the slope (low) and the sorption capacity of the sediments (relatively low).

Relatively high spatial impact scores for the saturated zone for the primary (coastal) aquifer indicate a high probability that contaminated water may move off-site before corrective action is taken. The relatively low persistence scores on the other hand suggest that groundwater at the site will not remain contaminated for a long time after the polluting activity has ceased (see also Appendix 7 .

The relatively high vulnerability of the CFA to contamination thus requires great care in assigning and protecting locations of groundwater abstraction for human consumption. It is recommended to establish set back distances for the Coastal Park waste disposal site to prevent impacts on livelihoods.

6.3 Comparison of vulnerabilities at the Coastal Park and Goedehoop sites

The unsaturated zone vulnerabilities are relatively high for both aquifers. From the smaller travel times and higher leaching potential indices as derived from the EUZIT spreadsheet tool and the UGIf model it can be concluded that the unsaturated zone vulnerability to dissolved organic contaminants (e.g. BTEX) of the primary Cape Flats aquifer at Coastal Park is higher than the vulnerability of the dual porosity, weathered zone aquifer at the Goedehoop site. This means that contaminants generated at the surface are likely to reach the water table and pollute the aquifer sooner at the Coastal Park waste disposal site.

The saturated zone vulnerability with respect to the spatial impact of inorganic and organic contamination is expected to be higher at the Coastal Park waste disposal site whereas the persistence is expected to be higher at the Goedehoop site. More detailed modelling, accounting for site specific physical properties, of the Cape Flats aquifer at the Coastal Park waste disposal site is needed to enable a better comparison of the saturated zone vulnerabilities of both aquifers.

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CHAPTER 7:

A FRAMEWORK TO SUPPORT DECISION-MAKING

7.1 Groundwater vulnerability in a South African context

Groundwater vulnerability assessments form an important input to managing the risk of water resource degradation. They aim at protecting groundwater quality by allowing development planners and regulators to incorporate a specific consideration of groundwater into their planning decisions (Appendix 4 ). In particular, it is a tool to assist with “the optimal distribution of future pollution sources” (Andersen and Gosk, 1987). Land-use planning that takes cognisance of impacts on groundwater could contribute significantly towards the sustainability of groundwater resources. Making a decision on where to locate or allow an activity, however, is complicated by the hidden nature of groundwater, and the complex heterogeneous setting in which it occurs, and therefore decision-making will benefit from a framework that supports decision making.

7.1.1 Water resource protection in South Africa

In South Africa, groundwater occurrence and use is widespread, but highly localised. It is physically and economically unfeasible to protect all groundwater resources to the same degree. Preventing all impacts on groundwater quality, would also not allow for the much needed social and economic development. The protection of groundwater resources will have to be prioritised according to:

- The value of the resource;
- The vulnerability of the resource; and
- The risk of adverse impacts on human health and ecosystems.

Land-use zoning is an effective method that restricts potentially polluting developments on important or sensitive aquifer systems. Water resource management agencies (i.e. DWAF and CMAs) must ensure that urban planners (in municipalities), for example, are aware of risks related to groundwater pollution and must encourage them to plan developments with due regard for the nations’ water resources. This requires that water resource management institutions (at national, provincial, regional and local levels):

- Participate in the evaluation of EIAs and intervene when impact assessments identify the potential for neglect or damage.

- Participate in land-use planning and strive to influence the planning so that activities with a high groundwater pollution risk are placed in areas with low or no groundwater potential.
- Enforce compulsory environmental management plans (including groundwater) for potentially polluting enterprises.

7.1.2 Water resource decision making

Water resource decision-making generates management actions that may not necessarily only address land use practices, but may target resource allocations, further data collection, and public behaviour. Decision-making, however, has to occur in the context of existing legislative and planning policy frameworks and societal values (e.g. environmental sustainability and the value of human life). Therefore, decision makers require appropriate understanding of the external decision-making environment in which they operate and the consequences of their decisions. This can be facilitated through the involvement of specialists, such as vulnerability assessment experts, in the decision-making process.

The Department of Water Affairs and Forestry (DWAF) has endeavoured to integrate Environmental Impact Assessment, in particular groundwater risk assessment, into the departmental decision making processes. To facilitate this an Environmental Management Framework was developed (DWAF 2002). It uses as its foundation a tiered approach (Figure 7.1), which recognises that, in an ideal sequence, Strategic Environmental Assessments (SEAs) should provide detail for project EIAs, which should aid the environmental management system (EMS) process.

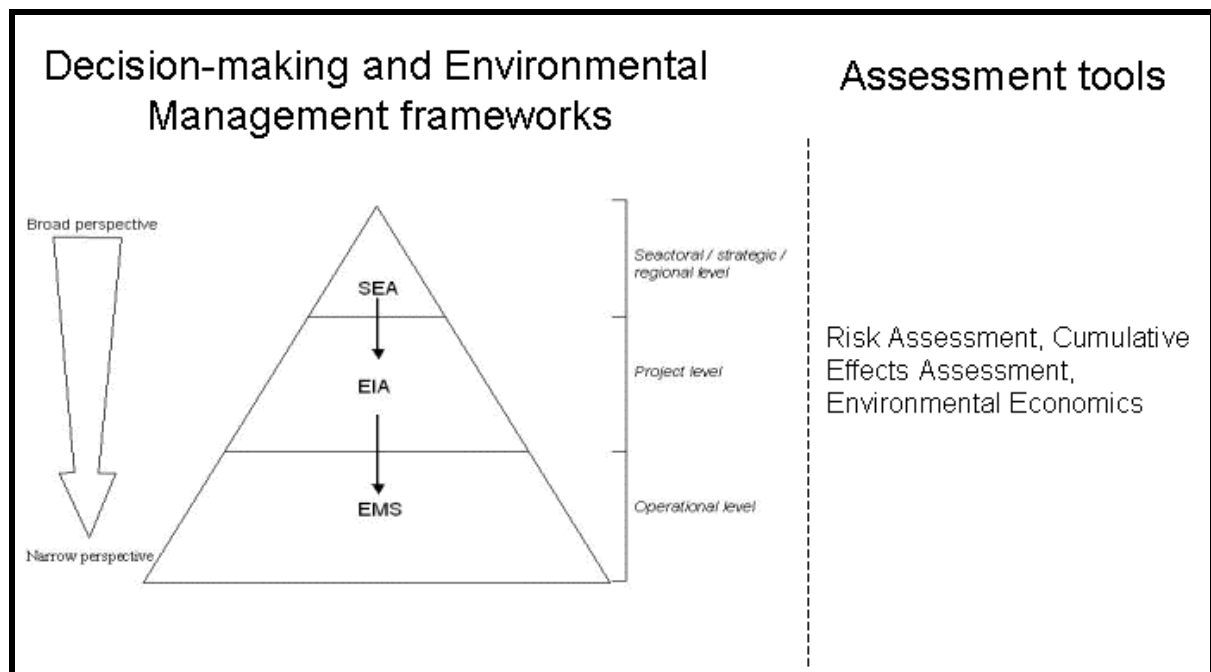


Figure 7.1: Hierarchy of Environmental Assessment and Management Tools (DWAF 2002).

Ideally, Strategic Environmental Assessments (SEAs) should be in place to indicate the limitations of project-specific EIAs. The Class of the aquifer (established through the National Classification System) should be used with the vulnerability to pollution, as input to strategic land-use decision making. Ultimately, human and ecosystem health concerns will determine the acceptability of pollution impact. These concerns can be assessed through a groundwater contamination risk assessment approach, such as that developed by Dennis et al. (2002). The contaminant risk assessment tool of Dennis et al. (2002) links to health and ecological risk assessment and cost-benefit analysis tools, and is founded on the premise that risk is a combination of (1) the probability that an adverse event will occur and (2) the consequences of that event.

7.1.3 Uncertainty in vulnerability assessments

The confidence with which the outputs of vulnerability assessments can be used in decision-making is directly related to the availability and quality of the data used, and the uncertainty or non-linearity in the relationships of the input parameters and the algorithms that integrate them. These factors have a significant influence on the uncertainty inherent in the vulnerability assessment outputs.

In many countries, uncertainty in environmental vulnerability is dealt with through the application in decision-making of the precautionary approach, especially where there is uncertainty on the level of harm an activity may cause to human health or the environment (EEA, 2001). This is done even if “some cause and effect relationships are not fully established scientifically” (Raffensperger, 1999). Among other things, the burden of proof is shifted to the proponent of an activity. The process of applying the precautionary principle must be open, informed and must include potentially affected parties.

Vulnerability assessments will always be subject to uncertainties albeit to a certain degree. Some of the uncertainties or errors can be quantified while others cannot. Statistical vulnerability methods in particular allow for the computation of the degree of uncertainty while index and overlay vulnerability methods do not always include any measures of uncertainty. One should at several stages re-evaluate the balance among increases in understanding of the system and resources needed in meeting science objectives while accounting for sources of uncertainty (Appendix 6 ).

Uncertainty in AVAPs' assessment approaches

The thickness of the soil zone has a large impact on vulnerability. To reduce the uncertainty in the result of an assessment, both hydraulic and chemical attenuation can be weighted over the whole depth of the unsaturated zone. For the unsaturated zone, variability in recharge and hydraulic conductivity mainly determine the uncertainty in the outcome of the assessments. A

sensitivity analysis of the outcome to changing key model parameters is a means to illustrate uncertainty in the results. Uncertainty or sensitivity analysis of the approaches developed for the saturated zone are more complex due to the large number of key parameters involved and the advanced modelling which is required. Nevertheless, the saturated zone approaches enable adequate comparison of vulnerabilities between different sites. For the GIS-based approach (UGIf) the sensitivity of model outcome to changing key parameters can be used to demonstrate the uncertainty in the approach.

7.2 AVAP in a decision-making context

The following main stages of an aquifer vulnerability decision support framework are defined (Figure 7.2):

- Stage I: Screening and Scoping – to determine whether an assessment of groundwater contamination risk is required for decision making;
- Stage II: Assessment – to determine the risk of groundwater contamination, which depends on the characteristics of the contaminant and the vulnerability of the aquifer to pollution; and
- Stage III: Decision-making – which integrates the outputs of the risk assessment into a cost benefit analysis, which the decision maker evaluates with consideration of relevant laws, regulations and guidelines and the principles and values of society.

7.2.1 STAGE I: Screening and scoping

Specialist groundwater input to the EIA process is required where the proposed activities may impact on groundwater resources. Of most relevance to the application of aquifer vulnerability assessments are activities “where effluent or chemicals with the potential to change groundwater quality is handled as part of the project, or discharged into the environment due to the project” (Saayman, 2005). A list of the sources of pollution/activities that most often impact on the quality of groundwater resources under South African conditions is given by Usher et al. (2004). This list should be used in conjunction with information on the presence of an aquifer and whether it is or may in future be of value (use) to society or to an ecosystem (see Figure 5-1). Examples of environmental settings that may induce an assessment of contamination risk / aquifer vulnerability are (modified from Saayman, 2005) include:

- The development utilises or will occur where it may impact an aquifer that is known (or suspected) to have significant exploitation potential.

Significance depends on factors such as water availability, water demand, and water quality.

- The development utilises or will occur where it may impact an aquifer that is the only (i.e. sole source aquifer) or a significant water supply source (or may become a significant water supply source) for an area utilised by a nearby community.

Especially where the aquifer supplies vulnerable or risk-prone communities. These are: communities whose reliance on water resource goods and/or services is particularly high. For example, communities who rely solely on groundwater for their water supplies; communities in dynamic, sensitive or harsh ecosystems, where extreme conditions (e.g. drought, floods, earthquakes, landslides) make them particularly vulnerable to additional negative impacts.

- A borehole used for any abstractive purpose occurs within the area of influence of the proposed development.

This area of influence will vary, depending on the hydrogeological setting and the nature of the development. It is suggested that a radius of 1 kilometre be used as an initial guideline of whether groundwater abstraction occurs near the proposed development. The greater the risk or impact associated with the pollutant release, the larger the screening radius should be.

- A wetland or sensitive ecological setting that is probably sustained by groundwater, occurs within the area of influence of the proposed development.

This area of influence will vary, depending on the hydrogeological setting and the nature of the development. It is suggested that a radius of 1 kilometre be used as an initial guideline of whether such ecosystems occur near the proposed development. Groundwater discharge to groundwater dependent ecosystems may be protected as part of the ecological reserve.

- Groundwater in the aquifer is to be managed to a 'good' or 'pristine' state.

This will be defined by the National Classification system that is being developed by the Department of Water Affairs and Forestry (DWAF) and will be set by the Minister. Some aquifers that are managed at lower levels may be allowed to perform some degree of natural attenuation (a licensed activity).

- Development will occur over an area where the release of toxic vapours (e.g. volatile organic compounds) from polluted groundwater is likely.

This type of pollution is usually associated with the release of petroleum products such as petrol and solvents used in dry cleaning and industrial processes.

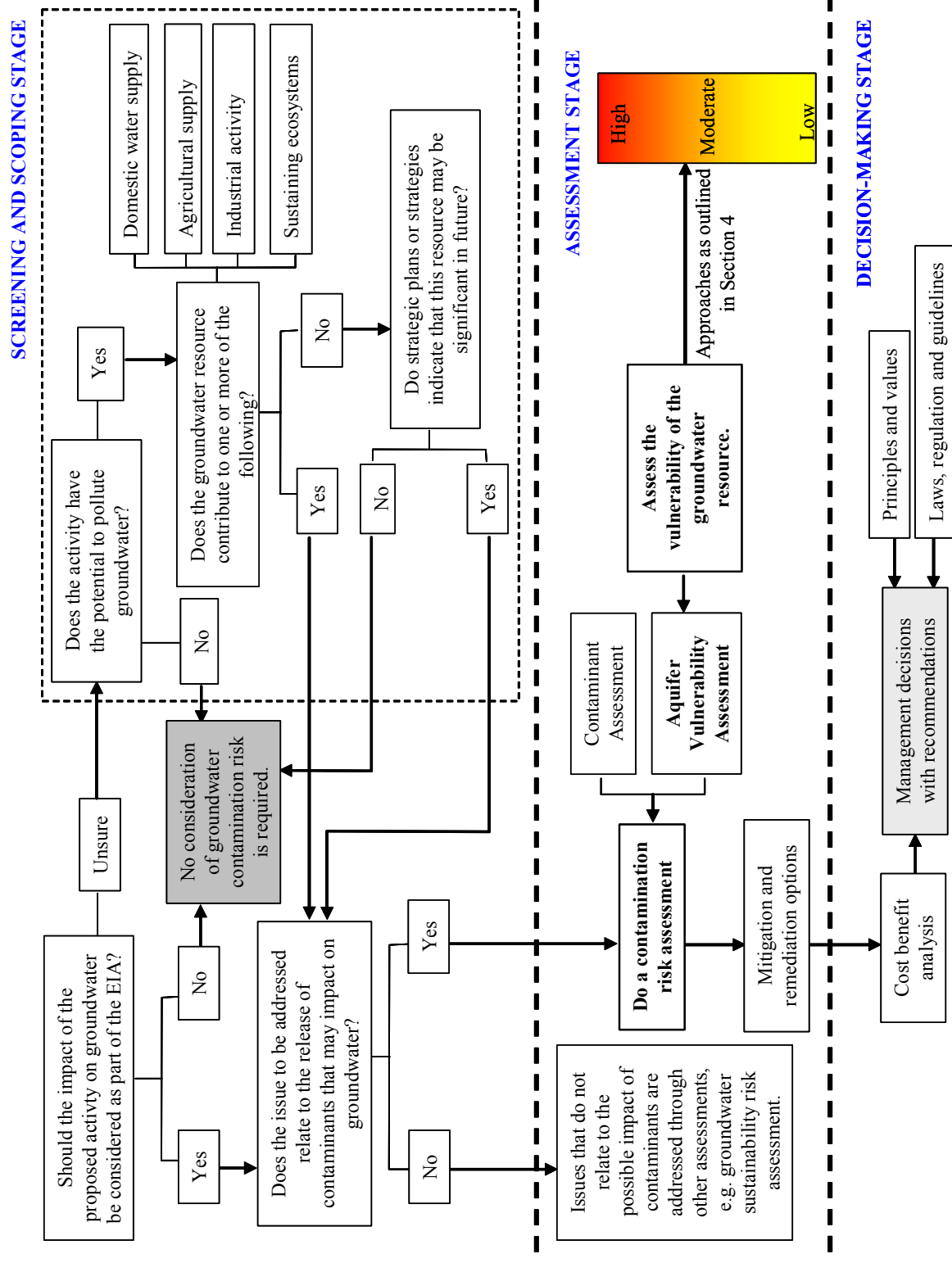


Figure 7.2: Schematic overview of aquifer vulnerability decision-making.

7.2.2 STAGE II: Vulnerability assessment

Where impacting activities and a sensitive environment coincide, some level of aquifer vulnerability assessment should form part of the EIA. The scale and the level of detail of the aquifer vulnerability assessment will depend on the scale of the proposed activity, sensitivity of the proposed location and expectation of adverse environmental impacts (Saayman, 2005).

Once it is determined that the assessment of groundwater vulnerability is required as part of the EIA process, the hydrogeologist will be faced with the question which aquifer vulnerability approach to follow. This choice is largely a function of the purpose of the assessment, such as:

- To enable land-use planning (i.e. a strategic assessment)

GIS overlay methods such as UGI_f are a means to getting an overview of aquifer vulnerability at a (sub)regional scale. Overlaying this with other development considerations (e.g. existing infrastructure and excluded areas) should enable decision makers to weigh the costs and benefits associated with particular land use options. The two methods require different types of data input, the availability which (or the lack thereof) may influence the choice of method.

- For a comparative assessment of two or more sites to establish their relative suitability for launching a development
- To establish the risk of groundwater pollution at a particular location/site.

The AVAP index methods provide a means to assessing aquifer vulnerability at a particular site. Depending on the type of activity envisaged, vulnerability assessments can be made for the soil, unsaturated zone as a whole and for the saturated zone. Vulnerability can be seen from different perspectives: from the soil zone as the first line of defence up to the saturated zone where both spatial ‘spreading’ and the persistence of a contaminant determine the aquifer’s vulnerability to contamination (see Chapter 4). Where the scale of the development and the associated risks are large, the vulnerability assessment approach that is selected may incorporate both GIS-based and zone specific index approaches.

A brief summary of the application of AVAPs’ vulnerability assessment methods is given in Table 7.1. The methods are grouped according to hydrologic zones and evaluated in terms of limitations, applicability and ratings (accuracy, ease of application and costs). The ratings are based on the experiences gained by AVAPs researchers and should only be used with care. Note that the AQUISOIL and EUZIT index approaches achieve essentially the same objective of assessing site specific vulnerability of groundwater to contamination, that is at the water table. With regards to the other approaches there is no limit to areal extent. Both AQUISOIL and EUZIT can be incorporated in a GIS.

7.2.3 STAGE III: Decision-making

Once the vulnerability assessment(s) have been completed, an evaluation needs to be made of the implications for groundwater resources and users of the resource. To a certain degree the index approaches do this, as the persistence in time and the spatial impact of the pollutant in the saturated zone. Likely input concentrations and load can be modelled to arrive at likely contaminant concentrations at the point of use.

Table 7.1: Overview of AVAPs' vulnerability assessment methods as applied to study areas.

Zone	Method	Limitations	Applicability	Rating ¹		
				Acc.	Ease	Cost
Unsaturated	AVRA (Aquifer Vulnerability Regolith Assessment)	Index method; soil properties such as pH, clay, organic matter and exchangeable cation content must be known for a meaningful vulnerability assessment	Site specific (m ²)	2	2	2
	EUZIT (Excel-based Unsaturated Zone Index Tool)	Index method; often assumed input parameter values; subjective weighting and rating		2	2	2
	UGIf (GIS-based) for dissolved organic contaminants	Heavy data requirements, time consuming. The model assumes steady state transport of pollutants. Individual pulses are not tackled.	No limitation on areal extent	1-2	3	3
Saturated	PHREEQC & MODFLOW for inorganic contaminants	Time consuming; heavy data requirements (aquifer hydraulics and geochemical characteristics and conditions); sensitive to boundary conditions		1-2	3	3
	PHT3D for BTEX					
	LNAPL Guide for BTEX from LNAPL pools	Considers only constant contaminant spill; no account of dilution by recharge; sensitive to boundary conditions		3	1	2
	BioChlor for chlorinated ethenes	Sensitive to boundary conditions				

¹ Accuracy rating: Class 1: difference from true value within a factor of 2, Class 2: within a factor of 5 and Class 3: within a factor of 10 or more; *Ease of application* is related to data requirements and data availability and is rated from 1: easy to use to 3: difficult to use; *Cost* is rated from 1: inexpensive to 3: expensive.

The findings of the vulnerability assessments form a basis for the formulation of management options and/or scenarios. These will form the starting point of the decision-making stage where analyses will be made of their costs and benefits and ultimately the formulation of management decisions and recommendations. Multi-stakeholder involvement is essential throughout the decision making process.

The options available for mitigating (preventing) the impact of pollution on water resources needs to be presented. This may include relocating the impacting activity to an area where impact is less likely or less significant. Often specialist input to the EIA occurs when significant investment has already been made into the location and design of a development. Project proponents are therefore encouraged to get specialist input as early as possible during the EIA process (see Saayman, 2005). An understanding of vulnerability will also provide valuable input on the design of groundwater quality monitoring systems, which may be stipulated as a condition of authorising a development.

The decision maker ultimately has the responsibility to weigh the costs associated with the mitigation of an impact on the environment against the likely costs of no action. Communication and feedback between the water-resource decision makers and scientists needs to continue during this stage of the decision making process to ensure that the results of the vulnerability assessments are correctly understood and the consequences of management decisions are clear.

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