THESIS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

Assessing Soil Functions for Sustainable Remediation of Contaminated Sites

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ABSTRACT

Soil contamination is a worldwide problem. Soil remediation is often carried out to reduce the risks posed by contaminants in the soil to human health and environment. Contaminant concentration is typically the only soil quality aspect maintained in remediation projects. However, emerging regulatory requirements on soil protection has introduced the soil function concept and demand that other chemical as well as physical and biological soil quality indicators are considered in soil management projects. Some remediation technologies may adversely impact soil functions, e.g. lead to compaction, nutrient deficiencies, and decreased water storage capacity. Others may lead to improvement of soil functions. Hence, it is important to evaluate the effects of remediation alternatives on soil functions when assessing the overall sustainability of decision options. A generic approach to soil function assessment in sustainability assessments is presented, conceptualizing linkages between soil functions, soil ecosystem services and the environmental, social and economic sustainability domains. A minimum set of soil quality indicators is identified and a scoring method for soil function assessment is developed, taking uncertainties of input data into consideration. The scoring method is further operationalized with the SF Box tool and integrated into SCORE (Sustainable Choice Of REmediation) for sustainability assessment of remediation alternatives. The developed soil function assessment method is applied on four case studies in Sweden. The results show that contaminated soil may have a good nutrient status and a good water storage capacity providing potentially favorable conditions for functioning, while reduction of the risks posed by contaminants to the environment does not necessarily lead to restoration of soil functions. To ensure proper soil functioning, special care needs to be taken with regard to physical, chemical and biological properties of the remediated soil in the top layer within future green areas.

Keywords: contaminated sites/soil, minimum data set, remediation, soil functions, soil ecosystem services, soil quality indicators, sustainability assessment.

LIST OF PAPERS

This thesis is based on the work contained in the following papers, referred to in the text by Roman numerals:

I. Volchko, Y., Norrman, J., Bergknut, M., Rosén, L., Söderqvist, T. (2013). Incorporating the Soil Function Concept into Sustainability Appraisal of Remediation Alternatives. *The Journal of Environmental Management,* 129, 367-376.

II. Volchko, Y., Norrman, J., Rosén, L., Norberg, T. (2014). A minimum data set for evaluating the ecological soil functions in remediation projects, accepted with minor revisions in *Journal of Soils and Sediments*.

III. Volchko, Y., Norrman, J., Rosén, L., Norberg, T. (2014). SF Box – a tool for evaluating the effects on soil functions in remediation projects, accepted with major revisions in *Integrated Environmental Assessment and Management*.

IV. Volchko, Y., Norrman, J., Rosén, L., Bergknut, M., Josefsson, S., Söderqvist, T., Norberg, T., Wiberg, K., Tysklind, M. (2014). Using soil function evaluation in multi criteria decision analysis for sustainability appraisal of remediation alternatives. *Science of the Total Environment*, published online, doi: 10.1016/j.scitotenv.2014.01.087.

V. Rosén, L., Back, P.-E., Söderqvist, T., Norrman, J., Brinkhoff, P., Norberg, T., Volchko, Y., Norin, M., Bergknut, M., Döberl, G. (2014). SCORE: Multi-Criteria Decision Analysis for Assessing the Sustainability of Remediation at Contaminated Sites, manuscript for submission to *Science of the Total Environment*.

Division of work between the authors:

Bergknut initiated the study in Paper I. All authors contributed to the suggested approach to soil function assessment within the MCDA for sustainability assessment of remediation alternatives. Volchko conceptualized the linkages between soil functions, ecosystem services and the sustainability domains, and performed the literature review on the effects of remediation on ecological soil functions. Volchko was the main author of the paper.

In Paper II, Volchko, Norrman and Rosén defined the aim and scope. Volchko derived the minimum set of soil quality indicators for soil function assessment, performed calculations and simulations. Norberg advised on uncertainty analysis. The results were analyzed by Volchko with support of all authors. Volchko wrote the main part of the paper.

In Paper III, Volchko developed the SF Box tool and performed calculations and simulations. The assessment results were analyzed by all authors. Volchko was the main author of the paper.

Paper IV was originally written by Volchko with support from Norrman and Rosén and revised by all authors. Volchko performed calculations and simulations. All authors analyzed the results. Volchko was the main author of the paper.

Rosén is the main author of Paper V. The presented SCORE method is based on the conjoint work of the research group reflected in the author list.

Publications not appended

In addition to the work presented in this thesis the author has published or contributed significantly to the following publications, which are not appended to the thesis:

Volchko, Y., Bergknut, M., Rosén, L., Norrman, J. (2011). Integrating the Soil Function Concept and Multi-Criteria Analysis for Sustainable Remediation of Contaminated Land, abstract, presentation, Sustainable remediation, Amherst, MA USA, June 1-3, 2011.

Norrman, J., **Volchko, Y.**, Rosén, L., Brinkhoff, P., Norin, M., Söderqvist, T., Kinell, G., Norberg, T. (2012). Development of a tool for evaluating the sustainability of remediation alternatives. In *Proceedings of the 16th Nordic Geotechnical Meeting*. Copenhagen, Denmark, May 9-12, 2012. Vol. 2/2, dgf-Bulletin 27, 793-800.

Volchko, Y., Bergknut, M., Rosén, L., Norrman, J., Söderqvist, T., Norberg, T. (2012). Accounting for soil functions and services in sustainability appraisal of remediation alternatives. In *Proceedings of the 4th Joint Nordic Meting on Remediation of Contaminated Sites*, short paper, oral presentation, Oslo, Norway, September 18-21, 2012.

Volchko, Y., Norrman, J., Bergknut, M., Rosén, L., Söderqvist, T. (2012). Markfunktioner – Hur kan vi bedöma effekter på markens funktioner av en sanering? Abstract, oral presentation, RenareMark Spring Meeting, Gothenburg, Sweden March 28-29, 2013.

Volchko, Y., Norrman, J., Rosén, L., Bergknut, M., Söderqvist, T., Norberg, T., Josefsson, S. (2013). Using soil function evaluation in multi criteria decision analysis for sustainability appraisal of remediation alternatives. In *Proceedings of the 12th International UFZ-Deltares Conference on Groundwater-Soil-Systems and Water Resource Management,* paper, poster presentation, Barcelona, Spain, April 16-19, 2013. Invited for publication in *Science of the Total Environment*.

Rosén, L., Back, P-E., Norrman, J., Söderqvist, T., Norberg, T., **Volchko, Y.**, Brinkhoff, P., Norin, M., Bergknut, M., Döberl, G. (2013). SCORE: Multi-Criteria Analysis (MCA) for Sustainability Appraisal of Remedial Alternatives. In *Proceedings of the Second International Symposium on Bioremediation and Sustainable Environmental Technologies*, June 10-13, 2013; Jacksonville, Florida, USA.

Volchko, Y. (2013). *SF Box – A tool for evaluating ecological soil functions in remediation projects.* Report 2013:1, ISSN 1652-9162, Chalmers Reproservice, Gothenburg, Sweden.

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I would like to extend my thanks to all my friends for staying in touch regardless of the distance. I am grateful to my parents Petro and Olga for their continuous support and encouragement. Дякую, мої рідненькі, за міцний фундамент в житті! I owe many thanks to my husband Sergei and my daughter Anastasia for their love and patience. Настенька и Сережка, спасибо за любовь и заботу!

Gothenburg,
Yevheniya Volchko

Table of contents

PAPERS I–V

Papers I-II are reprinted by permission of the publishers.

LIST OF NOTATIONS

Acronyms

AW	Available water capacity
BD	Bulk density
CBA	Cost-Benefit Analysis
CM	Content of coarse material
CP	Chlorophenol
EES	Ecosystem service
FAO	Food and Agriculture of United Nations
HC	Hazardous concentration
LOE	Line of evidence
MCDA	Multi-Criteria Decision Analysis
MDS	Minimum data set
MIFO	Method for inventory of contaminated areas
NOEC	No Observed Effect Concentration
OM	Organic matter content
P	Available phosphorus
PAF	Potentially affected fraction
SA	Sustainability assessment
SCORE	Sustainable Choice of REmediation
SF	Soil function
SIR	Substrate-induced respiration
SQI	Soil quality indicator
SSD	Species Sensitivity Distribution
ST	Soil texture
TOC	Total organic C
T-RFLP	Terminal restriction fragment length polymorphism
WTP	Willingness to pay

1 INTRODUCTION

The first chapter provides the background to the thesis. The aim and objectives are presented and the scope of the work is specified. Important limitations of the thesis are also presented.

1.1 Background

Soil contamination is a problem throughout the world. In Sweden alone, there are around 80 000 potentially contaminated sites (Swedish EPA, 2014). Remediation is usually carried out to break the polluter-receptor linkages and reduce the risks posed by contaminants to human health and the environment to allowable levels. Sometimes, remediation is driven by protection of the soil environment. In particular, this was the case for two-thirds of the remediation projects carried out in Sweden from 1998 to 2004 (Lundgren et al., 2006). In total, 80 remediation cases were analyzed covering 49 municipalities and 18 counties. One-fourth of the examined remediation projects were carried out in the municipalities of Malmö, Gothenburg and Stockholm, i.e. areas with a high degree of land utilization for construction purposes. Guideline values for protection of the soil environment reflect the contaminant concentration at which the soil is capable to carry out its functions relevant to land use (Swedish EPA, 2009). These values are typically derived from the Species Sensitivity Distribution (SSD) models, which are established under laboratory conditions, and take into consideration the effects of contaminants on the limited range of species and soil processes they mediate. However, the actual effects of contaminants on the soil environment in the field and those predicted with SSD models may differ. The Triad approach to ecological risk assessment is therefore suggested in order to account for contaminant concentrations, toxicity and effects of contaminants on the biota (e.g. effects on biodiversity function) (Swartjes et al., 2012b).

In order to ensure sustainable use of soil resources, the emerging regulatory requirements on soil protection introduce the soil function concept (COM, 2006). The proposed EU Soil Framework Directive lists soil functions and services that should be considered in soil management projects. The soil function concept demands a holistic view on soil quality in remediation projects, accounting not only for contaminant concentrations but also other chemical, physical and biological soil properties (Bone et al., 2010a, b). It is generally assumed that reduction of contaminant concentrations and amounts in the soil improves ecological soil functions (Swedish EPA, 1996, 2009). As a result, other soil quality aspects than contaminant concentrations are usually ignored in remediation projects. However, the remedial action itself can cause negative effects on the soil environment, e.g. lead to compaction, loss of organic matter, decline in biodiversity, and nutrient deficiency. For example, soil washing may adversely impact functions associated with primary production (Makino et al., 2007), electrokinetic treatments may affect both biodiversity function (Lear, 2007) and primary production function (Pazos et al., 2012). In contrast, immobilization of contaminants with amendments (Brown et al., 2005; van Herwijen et al., 2007) and phytoremediation (Doni et al., 2012; Epedle et al., 2008a; 2008b; 2009; 2010a; 2010b) can lead to risk reduction and simultaneous improvement of soil functions. Hence, it is important to account for the effects on soil functions when deciding on remediation alternatives. To fulfill remediation goals to protect the soil environment, it is essential not only to reduce the risks posed by contaminants to a soil biota but also to ensure reestablishment of favorable conditions in the remediated soil, enabling the biota to operate.

Soil functions form only one aspect of the overall sustainability assessment aiming to answer to what degree a remediation alternative contributes to sustainable development. Several international initiatives and national programs were launched for developing assessment frameworks and identifying important sustainability aspects/ criteria/ indicators that should be considered in remediation projects. The US EPA Green Remediation program resulted in development of metrics and a methodology for assessing environmental footprint of remedial actions (US EPA, 2012). The Sustainable Remediation Forum in the United Kingdom (SuRF UK) suggested a framework for sustainability assessment of remedial actions considering environmental, economic and social indicators (SuRF UK, 2010; 2011). The Network for Industrially Contaminated Land in Europe (NICOLE) also developed a framework for sustainability assessment in remediation projects (NICOLE, 2012). During 2004-2009 the Swedish EPA carried out a program comprising more than 50 projects on sustainable remediation. One of the outcomes of this program was a Multi Criteria Decision Analysis (MCDA)-based prototype for sustainability assessment of remediation alternatives (Rosén et al., 2009). This prototype was further developed into SCORE (Sustainable Choice Of REmediation) (Rosén et al., 2013; Paper V). SCORE for sustainability assessment of remediation alternatives has formed a basis for the work presented in this doctoral thesis.

1.2 Aim and objectives

The overall aim of this thesis was

> *to develop, apply and evaluate a method for incorporating the soil function concept into sustainability assessment of remediation alternatives.*

The specific objectives to fulfil the overall aim were to:

- develop a generic approach to soil function assessment in sustainability assessments;
- identify a minimum data set (MDS) and develop a method for soil function assessment;
- operationalize the soil function assessment method and integrate it into SCORE for sustainability assessment of remediation alternatives;
- practically apply and evaluate the developed soil function assessment method on case studies.

1.3 Scope of work

The main steps carried out within the scope of this project is presented in Figure 1.1. The first step in developing the generic approach to soil function assessment in sustainability assessments was to suggest a hierarchy between soil function and soil ecosystem services. This hierarchy links to the three domains of sustainability, i.e. environmental, socio-cultural and economic (Paper I).

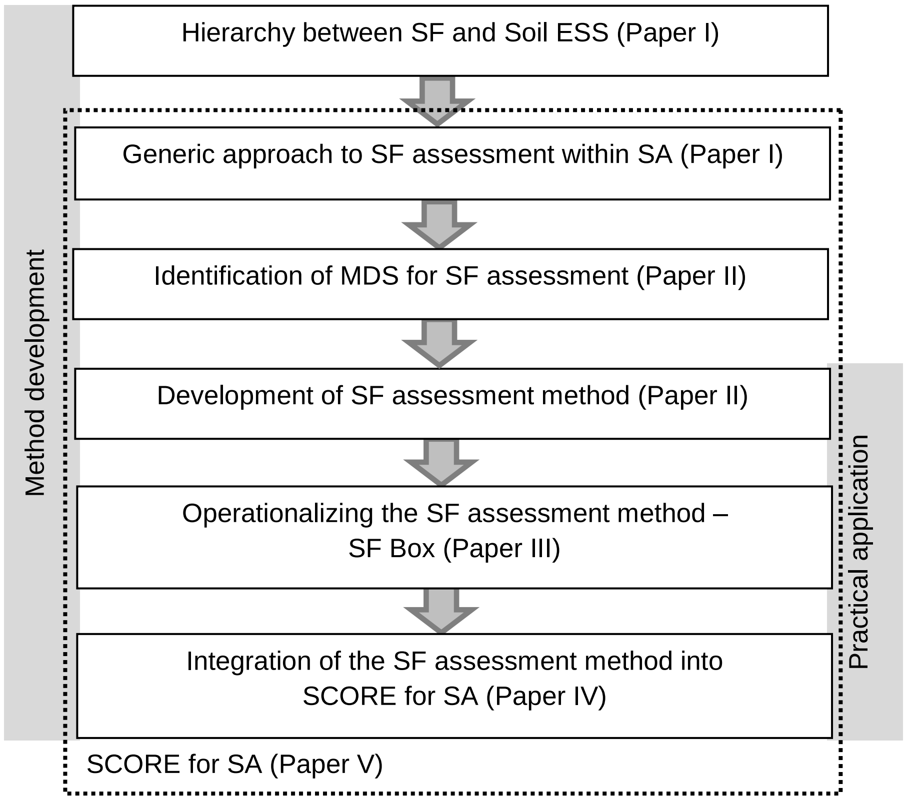


Figure 1.1 *The flow of the main steps carried out within the project. SF: soil functions, ESS: ecosystem services, SA: sustainability assessment, MDS: minimum data set.*

Based on the hierarchy, a generic approach to soil function assessment within sustainability assessment was developed using soil quality indicators (SQIs) in the environmental domain and soil service indicators in the socio-cultural and economic domains (Paper I). Further, a minimum set of SQIs, also referred to as MDS, was identified and a soil function assessment method was developed interpreting the performance of SQIs (Paper II). The SF Box tool was developed in order to operationalize the soil function assessment method (Paper III). The developed and operationalized method was integrated into SCORE for sustainability assessment of remediation alternatives (Paper IV). The soil function assessment method was practically applied and evaluated on case studies (Paper II-IV). Method development for soil function assessment was performed in the context of SCORE which is presented in Paper V.

An overview of the papers, including the title and the type of work, is presented in Table 1.1.

Table 1.1 Overview of five papers included in this thesis.

No	TITLE	TYPE OF WORK	STATUS
I	Incorporating the soil function concept into sustainability appraisal of remediation alternatives	Method development	Published
II	A minimum data set for evaluating the ecological soil functions in remediation projects	Method development and practical application	Accepted with minor revisions
III	SF Box – a tool for evaluating the effects on soil functions in remediation projects	Method development and practical application	Accepted with major revisions
IV	Using soil function evaluation in multi criteria decision analysis for sustainability appraisal of remediation alternatives	Method development and practical application	Published
V	SCORE: Multi-Criteria Decision Analysis for Assessing the Sustainability of Remediation at Contaminated Sites	Method development and practical application	Manuscript for submission

1.4 Limitations

Although the soil provides a multitude of functions, the developed soil function assessment method is limited to soil functions associated with primary production. These functions are only relevant to green areas within remediation sites. The method development is based on data available in the literature and not on laboratory studies.

2 THEORETICAL BACKGROUND

In this chapter the theoretical background to the contents of the thesis is presented.

2.1 Sustainable remediation

Published in 1987, the Brundtland report of the United Nations World Commission on Environment and Development entitled “Our Common Future” has served as an important catalyst for the worldwide appreciation for the idea of sustainable development. Industrialization, which took place in 20th century, resulted in overexploitation of natural resources and exhausted capabilities of ecosystems to absorb ever-increasing wastes. The Brundtland report recognizes that, in contrast to the rest of the world, people living in the developed countries use natural resources disproportionally creating intra-generational inequity. Furthermore, the increasing rate of use of these resources leads to inter-generational inequity hampering possibilities of the future generations to achieve a standard of living at least as good as that of the present. Therefore, the Bruntland report defines sustainable development as development that “meets the needs of the present without compromising the ability of future generations to meet their own needs” (WCED, 1987). Although there are different definitions of sustainable development in the literature, the essence is the same: such development should yield human well-being under conditions of intra- and intergenerational equity while preventing natural resources’ degradation.

The balanced interaction between the environmental, socio-cultural and economic domains (sometimes referred to as pillars or dimensions) of sustainability (or 3P representing Planet, People, and Profit) is usually used to operationalize the concept of sustainable development. In natural resource management projects, this concept is typically integrated into a management process by consistently assessing the effects of a planned action in the three sustainability domains (e.g. Harbottle et al., 2008; Rosén et al., 2009, 2013; Sparrevik et al., 2011; SuRF UK, 2010, 2011). Sometimes a management action may lead to trade-offs between the domains. However, a compensation of a negative change in a certain domain by a positive change in another one would lead towards weak sustainability (Ekins et al., 2003; van den Bergh, 2010). In contrast, a strong sustainability perspective implies that a management action must generate only positive changes in all three domains of sustainability without allowing for compensation.

The concept of sustainable development becomes a matter of growing interest in management projects of contaminated sites. Soil remediation is usually perceived as a sustainable action because it is designed to address contamination and reduce the risks posed by contaminants to human health and the environment. However, it can lead to both positive and negative impacts in the environmental, socio-cultural and economic domains. Sustainable remediation is therefore defined by SuRF-UK as “the practice of demonstrating, in terms of environmental, economic and social indicators, that the benefit of undertaking remediation is greater than its impact, and that the optimum remediation solution is selected through the use of a balanced decision-making process” (SuRF UK, 2010). Inspired by the concept of sustainable development, the US EPA defines green remediation as “the practice of considering all environmental effects of remedy implementation and incorporating options to minimize the environmental footprints of cleanup actions” (US EPA, 2012). The main principles of green remediation are to reduce energy use, increase the usage of energy from renewable resources, reduce air pollution and greenhouse gas emissions, reduce use of natural resources, decrease waste generation, and protect ecosystem services during site cleanup. The fundamental difference between sustainable remediation as defined by SuRF UK and green remediation is that the latter seeks to find the most environmentally-friendly option that achieves remediation objectives, while the former considers remediation as a part of broader sustainable development objectives (Brinkhoff, 2011).

2.2 Ecological risk assessment

Contaminant concentration is typically the only soil quality aspect maintained in soil remediation projects. In Sweden, soil quality standards are developed to handle three types of risks posed by contaminants in the soil: (1) human health risks, (2) risks to the soil environment, and (3) risks with regard to contaminant spreading to surface water and groundwater. The lowest contaminant concentration value among acceptable levels for the three risk types is used as a guideline value in a remediation project. Being typically the lowest, values for protection of the soil environment are often used, although the sites after soil treatment are planned to be utilized for construction purposes (Lundgren et al., 2006).

Risks posed to the soil environment are usually assessed by screening contaminant concentration in the soil and comparing them to guideline values derived from Species Sensitivity Distribution (SSD) models. This section provides a brief description of a SSD approach to ecological risk assessment, followed by the Triad approach which takes into consideration not only contaminant concentrations but also other important aspects of soil quality.

Species Sensitivity Distribution

Reflecting dose-effect relationships, SSD models form a basis for soil quality standards' development e.g. in the Netherlands and Sweden. A set of species (e.g. bacteria, earthworms, and plants) and processes (e.g. N mineralization, organic matter decomposition, and phosphatase activity) are exposed to different contaminant concentrations, doses and durations in order to evaluate the ecological effects (e.g. proportion dying, proportion germinating) on receptors. As a result, a cumulative distribution function (SSD curve) is built from a sample of toxicity data concerning a single compound and a set of different species and related soil processes (Figure 2.5). The SSD approach is used by selecting a maximum potential effect, e.g. 5% of species and processes (Y-axis in Figure 2.5), and then reading off the acceptable hazardous concentration (HC), e.g. HC5 (X-axis in Figure 2.5). HC5 is a hazardous concentration at which 5% of the tested species and processes would be exposed at or above No Observed Effect Concentration (NOEC).

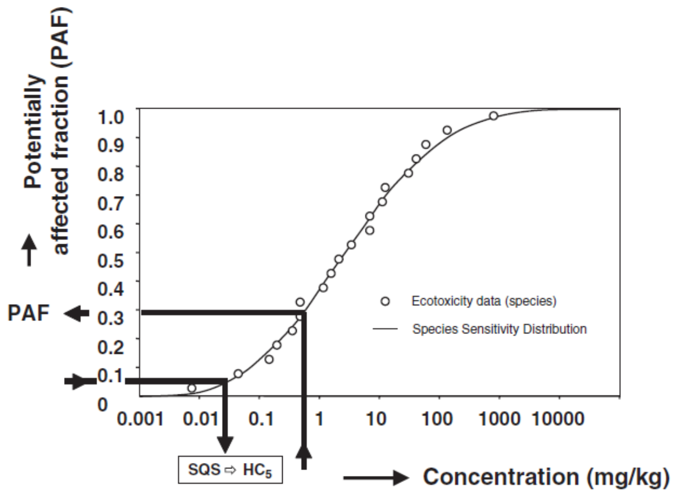


Figure 2.5 *Illustration of the species sensitivity distribution concept (Swartjes et al., 2012b). SQS – soil quality standard. HC_5 – hazardous concentration at which 5% of tested species are affected by the contaminant.*

In Sweden, HC25 and HC50 are used to develop guideline values for sensitive and less sensitive land uses respectively, implying that 75% and 50% of the tested species (and tested processes) would be protected from adverse impact posed by the compound. However, it should be mentioned that exceedance of e.g. HC25 does not necessarily mean actual loss of 75% of species in the field. The field conditions are likely to differ from the conditions in which the test data was established. Various confounding factors affect mobility and bioavailability of contaminants and thus toxicity (see e.g. Azarbad et al., 2012; Laskowski et al., 2003). For example, there is clear evidence that metals are more mobile and bioavailable in acidic soils than in neutral soils (Swartjes et al., 2012a; Tyler, 1992). Further, organic contaminants adsorb to soil organic matter (see e.g. Bergknut et al., 2010; Meijer et al., 2002; Meijer et al., 2003) and thus are less bioavailable in the soil rich in organic matter. In Sweden, the latter issue is addressed in the risk assessment model using corrections for organic carbon contents in the soil (Swedish EPA, 2009). Correction of the effects of organic matter and clay contents on mobility and bioavailability of metals are not taken into consideration in the Swedish risk assessment model as opposed to the Dutch model (Swartjes et al., 2012b). In the US EPA guidance on developing ecological screening values, factors affecting bioavailability of contaminants in the soil are taken into consideration (US EPA, 2003).

Triad approach

The Triad approach to ecological risk assessment is based on the simultaneous deployment of three independent types of assessments. This approach combines three lines of evidence (LOE): (i) chemistry – chemical analysis of contaminants and bioavailability analyses, (ii) ecotoxicology – effect assessments for species, soil processes and functions, and (iii) ecology – ecological status assessment.

The measurement endpoint in the chemistry LOE of the Triad risk assessment approach can be total contaminant concentrations in the soil and soil leachates, and potentially affected fraction (PAF). PAF is a percentage of species and processes potentially affected by contaminants and an extrapolated and corrected value derived from SSD models (Figure 2.5). When extrapolating, exposure data is typically corrected for differences in soil conditions (see e.g. de Zwarts et al., 2008; Swartjes et al, 2012b). These corrections often address bioavailability which implies that corrected PAF is lower than the uncorrected one. In contrast to evaluation of total contaminant concentration, bioavailability tests measure the bioavailable and mobile fraction of contaminants which has toxic effects on the exposed organisms (see ISO 17402 for description of methods). Hence, PAF can be extrapolated from SSD models using both bioavailable fraction of contaminants and total contaminant concentration with correction for soil conditions (Semenzin et al., 2008). Because of occurrence of contaminant mixtures, the SSD-based prediction of the ecological effects incorporates probable mixture impacts (the toxic pressure caused by the multi-substance PAF using the geometric mean) (Semenzin et al., 2008).

The measurement endpoints in the ecotoxicology LOE of the Triad risk assessment approach are usually survival rate, reproduction rate, replication rate, seed germination, and root elongation. The bioassays for sensitive species are usually used to evaluate bioavailability and toxicity of contaminants. The measurement endpoints in the ecology LOE are usually soil biological indicators (e.g. Semenzin et al., 2009; Chapman, 2013; Ribè et al., 2013). The ecology LOE of the Triad approach links the species to the processes and functions they mediate (Table 2.6). If particular species are affected by contaminants, the corresponding functions and processes are also considered to be impaired.

Table 2.6 The taxonomic group-ecological process-soil function relationships (represented with grey cells) accounted for in the Triad approach (after Semenzin et al., 2009).

TERRESTRIAL ECOSYSTEM														
		Biodiversity		Functional diversity										
				OM degradation		Recycling of nutrients					Soil detoxification	Water cycle		Formation of soil structure
Taxonomic groups	Ecological processes	Trophic chain complexity	Species of particular interest	OM decomposition and mineralization	Fragmentation and transformation of organic substances	N mineralization	Nitrification	Recycling of N	Recycling of P and C, gas exchange	N fixation	Soil detoxification	Evapotranspiration	Hydrological process regulation	Bioturbation and formation of soil aggregates
Microorganisms	Bacteria	■		■		■	■	■	■	■	■			
	Fungi	■		■		■		■	■		■			
	Protozoa	■												
Plants	Herbaceous species	■	■					■	■			■		
	Crop plants and ornamental species	■	■					■	■			■	■	
	Woody plants	■	■					■	■			■	■	
Invertebrates	Nematoda	■												■
	Enchytreids	■			■									■
	Earthworms (lumbricidae)	■			■								■	■
	Mites	■			■									
	Springtails	■			■									
	Macroarthropods (ants, termites)	■			■								■	■
Vertibrates	Mammals	■	■											
	Birds	■	■											
	Amfibians/reptiles	■	■											

2.3 Soil function assessment

The emerging regulatory requirements on soil protection demand a thorough assessment of soil functions in soil management projects. Sometimes soil functions are used to describe internal functioning of the soil ecosystem by means of soil quality indicators (e.g. Lehmann et al., 2008). However, sometimes soil functions are used interchangeably with ecosystem services to describe benefits humans gain from the soil ecosystem (e.g. de Groot, 2002). The proposed EU Soil Framework Directive combines both aspects of the soil function concept. First, this section compiles soil functions which are typically highlighted in the literature. Thereafter, a brief introduction to ecosystem services resulting from a collective action of soil, water, air and biota is provided. Further, selected ecosystem services where the soil is a main contributor or a driving force are compiled. Finally, the two complementary views on soil quality taken for soil function assessment are presented.

Soil functions

Soils provide multiple functions. This was first recognized by soil scientists in the late 70-ies (for historical background see Lehmann and Stahr, 2010) and by politicians more recently (COM, 2006). Several attempts have been made to group and classify the soil functions in order to better assess the effects of management actions on them (Table 2.1).

Table 2.1 Selected soil functions based on literature.

REFERENCE	SOIL FUNCTIONS
Andrews et al. (2004)	Nutrient cycling Water retention Physical stability and support Filtering and buffering toxic compounds Resistance and resilience of the soil ecosystem Biodiversity and habitat
Blum (2005)	Biomass production Protection of humans and the environment – Filtering, buffering and transformation of pollutants – Gas regulation (C sequestration) Gene reservoir Physical basis of human activities Source of raw materials Geogenic and cultural heritage

COM (2006)	Biomass production, including agriculture and forestry Storing, filtering and transforming nutrients, substances and water Biodiversity pool, such as habitats, species and genes Physical and cultural environment for humans and human activities Source of raw materials Acting as carbon pool Archive of geological and archeological heritage
de Groot et al. (2006)	Regulation function – Gas regulation (CO_2/O_2 balance) – Flood prevention – Water supply – Water regulation – Soil retention (roles of roots and soil biota) – Soil formation – Nutrient regulation – Waste treatment – Biological control (population control) Habitat function (for plants and animals) Production function – Food – Raw materials – Genetic resources – Medical resources – Ornamental resources Information function – Aesthetic information – Recreation – Cultural and artistic information – Spiritual and historic information – Science and education Carrier function – Habitation (living space for humans) – Cultivation (food production and raw material extraction)
Kibblewhite et al. (2008)	C transformation Nutrient cycling Soil structure maintenance Biological population regulation
Lehmann et al. (2008)	Basis and habitat of human life Basis for life and habitat of flora and fauna Storage-, filtration- and transformation-medium – Component of water cycle – Component of nutrient cycle – Filter and buffer of heavy metals – Transformation medium (turnover of chemical substances by soil microorganisms) Production site for food and other biomass – Grassland use production – Wheat production Archive – Archive of natural history – Archive of cultural history

Semenzin et al. (2009)	Biodiversity Organic matter degradation Recycling of nutrients Soil detoxification Water cycle Formation of soil structure
Singer and Ewing (2000)	Maintaining biological activity/productivity Serving as a medium for plant/crop growth Support for plant productivity/yield Support for human/animal health Partitioning and regulating water/solute flow Serving as an environmental buffer/filter Maintaining environmental quality Cycling nutrients, water, energy, and other elements
Weber (2007)	Production function Carrier function (bearing traffic and buildings) Filter, buffer and reactor function Resource function (base materials for industry) Habitat function (for flora and fauna) Cultural and historic function Climate regulation function (C storage) Regulating water storage and evapotranspiration

Ecosystem services

It is generally agreed that ecosystem services are the benefits humans gain from ecosystems (MA, 2005). Ecosystem functions result in ecosystem services once they are delivered to and utilized by a society to yield human well-being (Costanza et al., 1987; de Groot et. al, 1992, 2002, 2006). Recently, ecosystem services were defined as the beneficial flows arising from natural capital stocks (e.g. soils, forests, water bodies) and fulfilling human needs (Dominati et al., 2010). The Millennium Ecosystem Assessment (MA, 2005) classifies ecosystem services into provisioning (e.g. food, fresh water, wood and fiber), regulating (e.g. climate regulation, flood regulation, water purification), cultural (e.g. spiritual, aesthetic, recreational aspects), and supporting services (e.g. soil formation, nutrient cycling, primary production) (Figure 2.1). The first three categories of services directly affect people, whereas supporting services maintain the other services. One-to-one matches between functions and services are unusual, as a single ecosystem service may result from several ecosystem functions and vice versa (Costanza et al., 1987; MA, 2005). Some ecosystem services can become ecosystem goods in the market place.

Although authors agree that ecosystems deliver ecosystem services to produce human well-being, the nature of these services is a topic of debate in the literature. Dominati et al. (2010) highlight a controversy that revolved around ecosystem functions and processes used for defining the ecosystem services

(Fisher and Turner, 2008; Wallace, 2007). Wallace (2007) suggests using ecosystem functions synonymously to ecosystem processes as already done in soil science (e.g. Barrios et al., 2007; Kibblewhite et al., 2008; Lavelle et al., 2006).

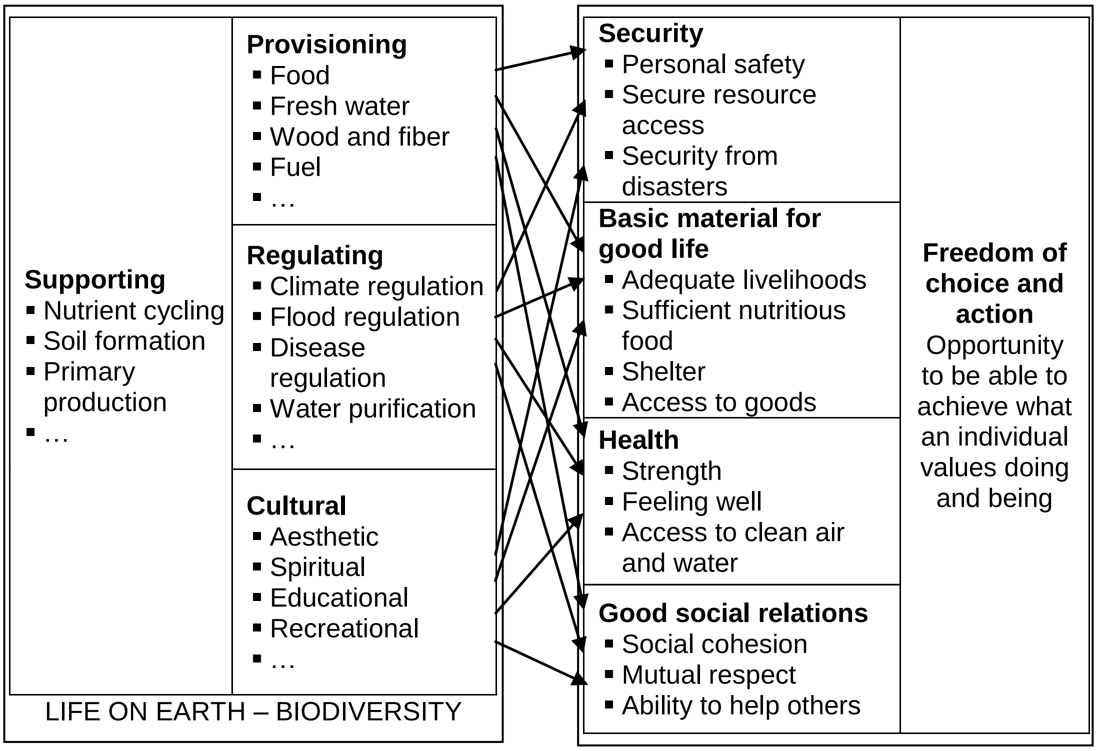


Figure 2.1 *The relationships between the ecosystem services and constituents of human well-being (MA, 2005).*

Fisher and Turner (2008) argue, contrary to MA (2005) and Wallace (2007), that services are not benefits but functions and/or processes once they are directly or indirectly utilized by an individual or a society. Fisher et al. (2009) suggest that ecosystem services include ecosystem organization, structure, processes and functions if they are passively or actively consumed by humans.

Soil ecosystem services

Ecosystem services result from complex interactions between air, water, soil and biota through the universal driving forces of matter and energy. An ecosystem service where the soil is a main contributor is called a soil ecosystem service. Some examples of soil ecosystem services are provided in Table 2.2.

Table 2.2 Selected soil ecosystem services.

REFERENCE	SOIL ECOSYSTEM SERVICE
Barrios et al. (2007)	Nutrient uptake Nutrient cycling Regulation of soil erosion Carbon sequestration Water flow and storage Biological control of pests and diseases
Daily (1997)	Water flow and retention Physical support for vegetation Retention and cycling of nutrients Disposal of wastes and dead organic matter Regulation of major element cycles Maintenance of biodiversity and habitats
de Groot (2006)	Maintenance of good air quality Flood prevention Drainage and natural irrigation Maintenance of arable land Protection from erosion/saltation Maintenance of productivity on arable land Maintenance of natural productive land Pollution control/detoxification Control of pests and diseases Maintenance of biological and genetic diversity Food production (e.g. gathering of fruits, farming) Production of drugs and pharmaceuticals Provision of drinking water Provision of raw materials for building and manufacturing Provision of living space for humans Provision of living space for wild plants and animals Provision of space for solid waste disposal Enjoyment of attractive landscape features Heritage value of natural ecosystems and features Use of nature for scientific research and education
Dominati et al. (2010)	Cultural services – Spirituality – Knowledge – Sense of place – Aesthetics Regulation services – Flood mitigation – Filtering of nutrients – Biological control of pests and diseases – Recycling of wastes and detoxification – Carbon storage and regulation of NO_2 and CH_4 Provisioning services – Provision of physical support – Provision of food, wood and fiber – Provision of raw materials
Lavelle et al. (2006)	Production services – Water supply Support services – Nutrient cycling

− Soil formation − Primary production Regulation services − Flood and erosion control − Climate regulation

Holistic view on soil quality

Soil quality indicators are typically used for soil function assessment. The soil quality concept is usually used to describe the capacity of the soil to (1) function, e.g. basis for primary productivity and nitrogen cycling, and (2) perform according to its purpose (end use), e.g. crop production. There is no consensus on the definition of soil quality in the literature (see compilation of definitions in Bone et al., 2010a). The most frequently cited definition of soil quality is “the capacity of a soil to function, within ecosystem and land use boundaries, to sustain productivity, maintain environmental quality, and promote plant and animal health” (Doran and Parkin, 1994). In recent years, the term “soil quality” has been redefined introducing a new term, “soil health”, to place more emphasis on the soil “as a living and dynamic system whose functions are mediated by a diversity of soil organisms” (Doran and Zeiss, 2000). The soil health paradigm holds a holistic view on soil quality by integrating three soil quality elements: physical, chemical and biological (Doran and Zeiss, 2000; Karlen et al., 2003; Schindelbeck et al., 2008). Incorporation of the soil functions into definition of soil quality is not universally accepted. For example, Letey et al. (2003) and Sojka and Upchurch (1999) emphasize that soil quality should be evaluated relative to the end use of the soil.

For detailed review of physical, chemical and biological soil quality indicators the reader is referred to the work by Kruse (2007). A review of the SQIs which are used for derivation of multiparametric soil quality indices for agricultural soils are presented in Bastida et al. (2008). The most frequently used SQIs for agricultural purposes are organic matter, organic carbon, bulk density, aggregate stability, pH, electric conductivity (or salinity), forms of nitrogen, microbial biomass, and respiration. There are no unified MDS for soil function assessment, because each soil function will require a unique set of SQIs (Lehmann et al., 2010). On the other hand, a single SQI can capture several soil processes (see Table 2.4) and several soil functions (see Table 2.5). Andrews et al. (2004) suggest six sets of potential SQIs relevant to six soil functions corresponding to different soil management goals (Table 2.3).

Table 2.3 A set of potential soil quality indicators for soil function evaluation (based on Andrews et al., 2004).

SOIL FUNCTIONS	SOIL QUALITY INDICATORS	MANAGEMENT GOAL
Biodiversity and habitat	– Nematode maturity index – qCO_2 (metabolic quotient; respiration to microbial biomass ratio)	Environmental protection
Filtering and buffering	– Bulk density – Phosphorus – Total organic carbon	Waste management and environmental protection
Nutrient cycling	– Microbial biomass carbon – Potentially mineralizable N – pH – Phosphorus	Productivity, waste management, environmental protection
Physical stability and support	– Macroaggregate stability – Bulk density – pH	Productivity, environmental protection
Resistance and resilience	– Soil depth – Total organic carbon	Productivity, waste management, environmental protection
Water relations	– Available water capacity – Bulk density – Electric conductivity – Sodium absorption ratio – pH	Productivity, waste management, environmental protection

Based on literature studies and statistical analysis of more than 1500 soil samples, Gugino et al. (2008), Idowu et al. (2008) and Schindelbeck et al. (2008) suggest 12 physical, chemical and biological SQIs (out of 39 tested) to be used for soil health assessment capturing soil processes related to crop production (Table 2.4).

Table 2.4 Soil quality indicators for assessment of soil functional processes related to crop production (Idowu et al., 2008).

SOIL QUALITY INDICATOR	SOIL FUNCTIONAL PROCESS
Soil texture and stone content	All
Aggregate stability	Aeration, infiltration, shallow rooting, crusting
Available water capacity	Plant-available water retention
Soil strength (penetrometer)	Rooting
Organic matter content	Energy/C storage, water and nutrient retention
Active carbon content	Organic material to support biological functions
Potentially mineralizable N	Ability of microorganisms to supply nitrogen
Root health rating	Soil-borne pest pressure
pH	Toxicity, nutrient availability
Extractable phosphorus	Phosphorus availability, environmental loss potential
Extractable potassium	Potassium availability
Minor element contents	Micronutrient availability, elemental imbalances, toxicity

Lehmann et al. (2008) suggest seven sets of SQIs to assess seven soil functions: (1) basis for habitat of flora and fauna, (2) component of water cycle, (3) component of nutrient cycle, (4) filter and buffer of heavy metals, (5) transformation medium, (6) grassland use production, and (7) wheat production (Table 2.5).

Table 2.5 Soil quality indicators used for soil function evaluation (based on Lehmann et al., 2008). Grey cells indicate relevance of soil quality indicators to soil functions.

	SOIL FUNCTIONS						
SOIL QUALITY INDICATORS	Basis for life and habitat of flora and fauna	Component of water cycle	Component of nutrient cycle	Filter and buffer of heavy metals	Transformation medium	Grassland use production	Wheat production
Soil texture	■	■	■			■	■
OM content	■	■		■	■	■	■
Bulk density	■	■	■			■	■
Available field capacity	■	■				■	■
Depth of horizon	■	■	■	■		■	
Content of coarse material	■	■	■	■		■	
Clay content		■		■			■
Groundwater level	■				■		
Electrical conductivity	■						
Soil structure					■	■	
Saturated hydraulic conductivity		■					
Air capacity		■	■			■	■
Cation exchange capacity			■			■	■
Aggregation				■			
pH			■	■	■		
Potential rooting depth						■	■
Average annual temperature						■	■
Slope gradient		■					■
Redoximorphic features			■				

Soil biology perspective

The "soil biology" view holds that the identity and roles of each soil organism is vital for proper functioning of an ecosystem. Soil organisms can be grouped according to their size (taxonomic groups) or according to their roles in the ecosystem (functional groups). Further, functional groups can be merged into functional assemblages, e.g. decomposers, nutrient transformers, ecosystem engineers, and bio-controllers (Figure 2.2). These assemblages can in turn be linked to four aggregated ecosystem functions: (1) carbon (C) transformation, (2) nutrient cycling, (3) soil structure maintenance, and (4) biological population regulation.

Decomposition of organic matter is accompanied with C transformation in litter (i.e. dead plant material) and other organic inputs through feeding activities (i.e. fragmentation and enzymatic activity) of a diverse suite of soil decomposers. Controls over the activities of these organisms are therefore usually studied to better understand controls over soil organic matter decomposition (Chapin et al., 2012). Strongly linked to the decomposition of organic matter, the cycling of nutrients is mediated by nutrient transformers as well as decomposers (Figure 2.2). Through combined action of plant roots and soil organisms, known as "ecosystem engineers", the soil is modified, creating aggregates, pores and channels and thus providing microhabitats for other organisms (Barrios et al., 2012). Being carried out through competition, predation, and parasitism, biological population regulation is an important function of the bio-controllers, leading to population control and disease suppression in the soil (Barrios et al., 2012). These aggregate ecosystem functions are further linked to the soil processes and the related soil ecosystem goods and services (Figure 2.2).

Biological soil quality indicators are usually used to measure biodiversity and ecosystem functions mediated by soil organisms. For example, various biodiversity indices were developed to quantify microbial diversity, e.g. Shannon diversity index (species diversity and composition) (Shannon and Weaver, 1949), Margalef diversity index (species richness) (Margalef, 1958), Pielou diversity index (species evenness) (Pielou, 1975). Such quantification became possible thanks to the research advances in recent decades. These advances have resulted in a set of advanced methods to study soil microbial communities, e.g. community level physiological profiling (CLPP) based on short-term responses to the addition of carbon substrates, or 16S rRNA gene based terminal restriction fragment length polymorphism (T-RFLP). Also, different methods have been developed to study community structure of the larger organisms (see review of standard methods in Römbke et al., 2006).

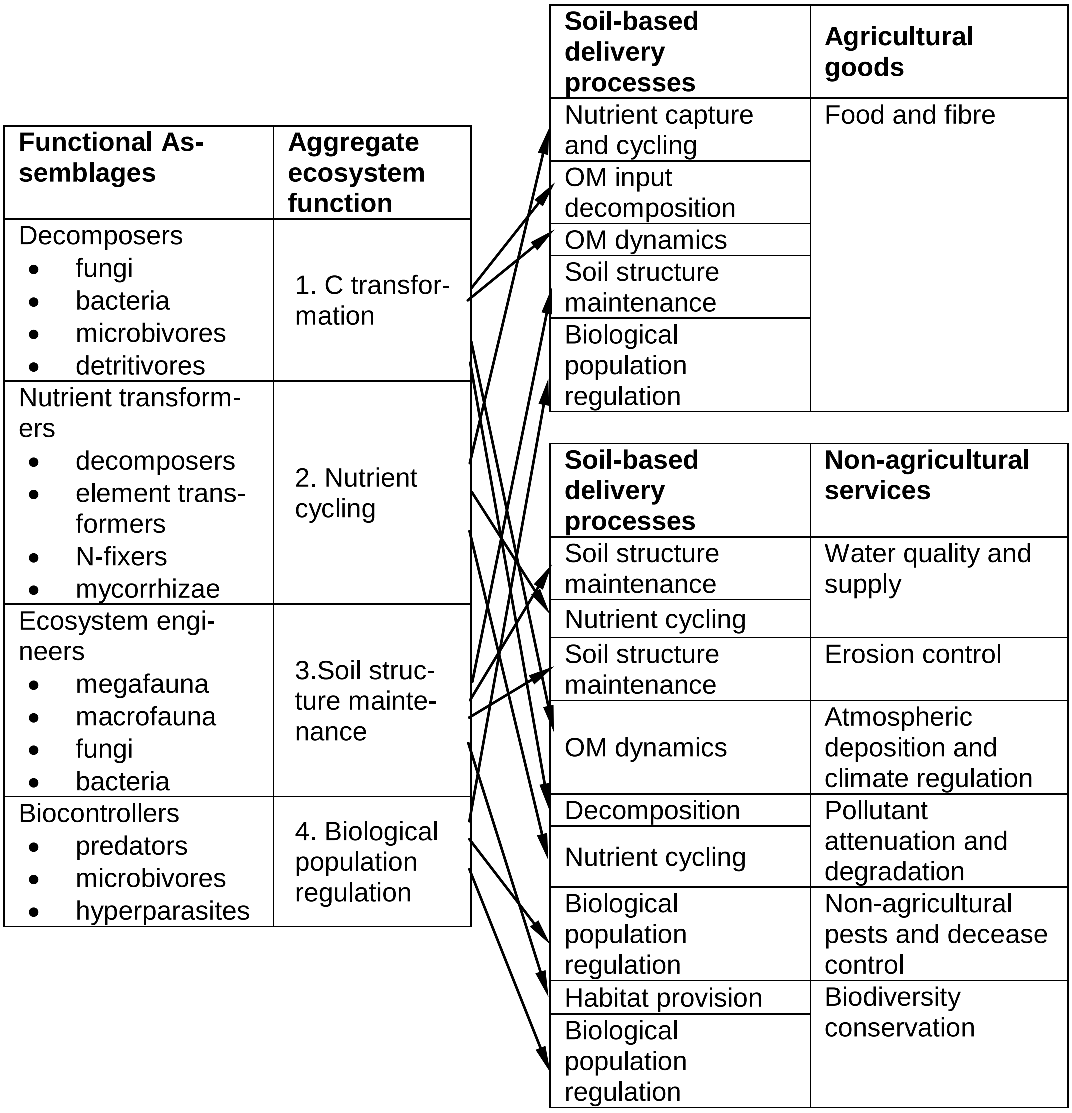


Figure 2.2 Conceptual framework of linkages between soil biota, biologically-mediated processes and the provision of soil ecosystem goods and services (after Barrios et al., 2012; originally modified from Kibblewhite et al., 2008).

There is no standardized minimum set of biological SQIs for assessment of the effects on ecosystem functions, because different assessment goals would result in different measurement endpoints. Faber et al. (2013) grouped the most frequently used biological SQIs into four major groups: (*i*) microbes, (*ii*) fauna, (*iii*) processes and (*iv*) "-omics" (i.e. molecular fingerprinting of soil microbial communities) (Table 2.3).

Table 2.3 Biological soil quality indicators used in approximately 14 200 measurements in European soils (after Faber et al., 2013). PLFA – phospholipid-derived fatty acids; SIR – substrate-induced respiration; T-RFLP – terminal restriction fragment length polymorphism; amoA – amoA genes in archaea (coding for the alpha-subunit of the ammonia monooxygenase); ARISA - automated rRNA intergenic spacer analysis fingerprints; ITS – Internally transcribed spacer sequences.

FAUNA
Nematodes
Micro-arthropods
Isopods
Enchytraeids
Earthworms
Ants
MICROBES
Bacterial activity
Fungi
Bacterial biomass + SIR
Protozoans
PROCESSES
(Basal) respiration + C mineralization
Nitrification (ammonium oxidation), N mineralization (anaerobic N)
Enzyme activities
Bait lamina
OMICS
PLFA microorganisms
Bacterial functional diversity
Bacterial structural diversity
Fungi F-ARISA
Bacteria B-ARISA
Archea (amoA)
Arbuscular mycorrhizae 18S T-RFLP
Fungi ITS T-RFLP

Nematodes, soil microbial biomass (including substrate-induced respiration, SIR), basal respiration (including potential C mineralization), ARISA – automated rRNA intergenic spacer analysis fingerprints have been the most frequently used biological indicators for soil monitoring purposes (Faber et al., 2013).

Using expert opinions and a multi-tier sieving approach, the study by Ritz et al. (2009) derives the potential biological indicators relevant to three functional categories: (1) food and fiber production, (2) environmental interactions and (3) supporting habitat and biodiversity. The identified indicators include (a) soil microbial taxa and community structure using T-RFLP-based approaches (ISO 11063:2012); (b) soil microbial community structure and biomass from phospholipid fatty acids (PLFA) (ISO/TC 29843-2:2011); (c) soil respiration and C cycling from multiple SIR (ISO 16072:2002); d) biochemical processes from multi-enzyme profiling (ISO/TS 22939:2010); (e) nematodes (ISO 23611-4:2007); (f) microarthropods (ISO 23611-2:2006); (g) on-site visual recording of soil fauna and flora; and (h) pitfall traps for ground-dwelling and soil invertebrates. The standards for analysis of the majority of these indicators are developed by International Standard Organization (ISO).

Such profiling technique for the gene-based study as T-RFLP has proven useful in the monitoring of a microbial community during bioremediation (Hackl et al. 2012; Vázquez et al. 2009), electrokinetic treatment of the contaminated soil (Pazos et al., 2012) and soil washing (Jelusic et al., 2013). By mapping the genetic structure it is possible to analyze whether the contaminated soil can be stimulated and recovered. Enzyme profiling and SIR have also been successfully used for monitoring the microbial diversity in the contaminated soil during phytoremediation (Epelde et al. 2008a; 2008b; 2009; 2010a; 2010b) and electrokinetic treatment (Pazos et al. 2012).

3 METHODS

This chapter includes a general description of the underlying methods and techniques used in this thesis.

3.1 The SCORE method

SCORE is an MCDA-based method that aids a decision-maker in comparing available remediation alternatives by consistently evaluating to what degree they fulfil a set of performance criteria in the environmental, socio-cultural and economic domains. The SCORE method for sustainability assessment underpins the work presented in Papers I-IV and is described in Paper V.

SCORE uses an MCDA approach, which is increasingly suggested for sustainability assessment of remedial actions (e.g. Harbottle et al., 2008; Rosén et al., 2009; Linkov and Moberg, 2011; Brinkhoff, 2011; Sparrevik et al., 2012). SCORE includes: (1) criteria selection, (2) evaluation of the remediation alternatives against criteria in the environmental, socio-cultural and economic domains, (3) criteria weighting (i.e. identifying their relative importance), (4) information synthesis, comparison of remediation alternatives based on their overall performance on the criteria, and (5) sensitivity and uncertainty analyses of the obtained results (Figure 3.1). SCORE helps a decision-maker to establish preferences between remediation alternatives by reference to explicit set of criteria representing the three domains of sustainability (Table 3.1).

SCORE is aimed at evaluating changes (effects) as a result of remediation relative to a reference alternative. It is up to a decision-maker to define the reference alternative. Typically, it is a base case scenario when no remedial action is taken for reduction of the risks posed by contaminants to human health and the environment.

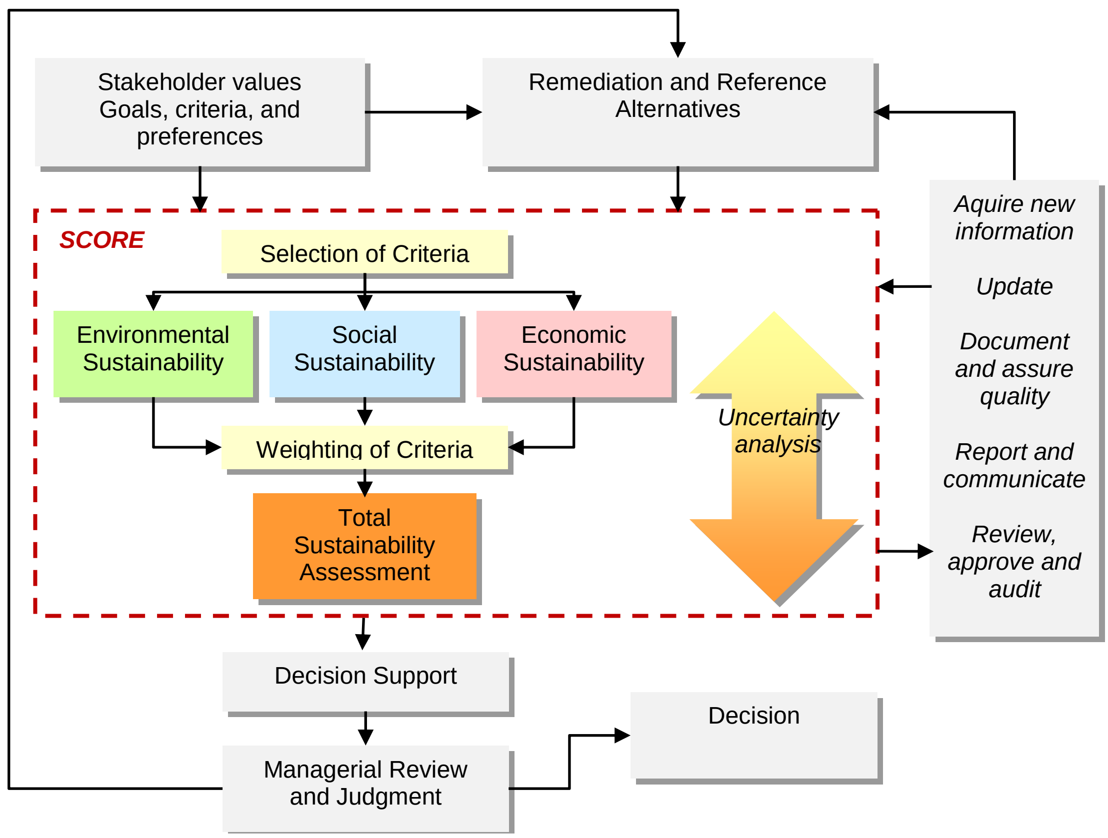


Figure 3.1 SCORE for sustainability assessment of remediation alternatives (Rosén et al., 2014).

The effects in the environmental and socio-cultural domains are scored as follows: Very positive effect: +6 to +10; Positive effect: +1 to +5; No effect: 0; Negative effect: -1 to -5; Very negative effect: -6 to -10. The social profitability criterion of the economic domain is addressed with a Cost Benefit Analysis (CBA) (Rosén et al., 2008).

Table 3.1 Key performance criteria for sustainability assessment in remediation projects (Rosén et al., 2013).

ENVIRONMENTAL DOMAIN	SOCIO-CULTURAL DOMAIN	ECONOMIC DOMAIN
• Soil • Flora and fauna • Groundwater • Surface water • Sediment • Air • Non-renewable natural resources • Non-recyclable waste	• Local environmental quality and amenity • Cultural heritage • Equity • Health and safety • Local participation • Local acceptance	• Social profitability

The SCORE is based on a liner-additive model (CLG, 2009):

$$s_j = \sum_m w_m s_{jm} \tag{3.1}$$

where s_{jm} is the score for j-th alternative and m-th criterion and w_m is the weight determining the relative importance of each criterion. This model is only justifiable if the criteria are mutually independent, i.e. the score assigned to one criterion does not depend on scores assigned to other criteria.

Criteria for all three sustainability domains are evaluated with respect to effects on-site and off-site as well as effects due to reduction in source contamination and due to the remedial activity itself. A normalized sustainability index integrates effects in the environmental and the socio-cultural domains of sustainability with assessment of social profitability in the economic domain. The most sustainable alternative is the one which generates the highest sustainability index.

Uncertainties in scores for the criteria of the environmental and the socio-cultural domains and in results of CBA for the social profitability criterion of the economic domain are treated with Monte Carlo simulation. The assignment of the uncertainty distributions is performed in three steps: (1) selection of range of effects, i.e. selection of whether all types of effects, only positive, or only negative effects are possible for the specific criterion; (2) estimation of the most likely effect describing the expected effect, i.e. scores in interval between -10 and +10 and the monetized costs and benefits; and (3) assigning the uncertainty level of the estimation of the most likely effect (Rosén et al., 2014). The three-step procedure results in a probability distribution representing uncertainties of inputs to the sustainability assessment. The resulting uncertainty of the sustainability assessment is calculated by means of Monte Carlo simulation.

Since aggregation of each option's performance across the criteria can lead to compensation of good performance on one criterion for weaker performance on another, the SCORE allows for analysis of trade-offs between different criteria. If the remediation alternative generates a positive sustainability index, it is regarded as leading towards weak or strong sustainability. It is considered as leading towards strong sustainability if it performs positively on all criteria, i.e. without allowing for compensation among them.

3.2 Soil function assessment

Scoring soil quality indicators

A scoring method is used to transform the input values of soil quality indicators into the fractional numbers to integrate information on the soil quality and aid the decision making process on the management action. The method was used in the work presented in Papers II-IV.

The scoring method was initially described by Andrews et al. (2004) and followed by Gugino et al. (2008), Idowu et al. (2008), Schindelbeck et al. (2008) and Volchko (2013). Scoring is performed in three steps: (1) selection of a minimum data set, (2) interpretation of indicators and (3) calculation of soil quality index (Figure 3.2). In order to interpret the measured values of soil quality indicators, three types of scoring curves are suggested, i.e. “more is better”, “optimum”, and “less is better” (i.e. shapes of curves in the interpretation of indicators step; Figure 3.2). For the “more is better” example, the higher the value of the SQI, the higher the sub-score of this indicator. For the “less is better” example, the lower the value of the SQI, the higher the sub-score. For the “optimum” example, there is a limited range of values corresponding to high sub-scores, whereas “less” and “more” than these optimum values are scored lower.

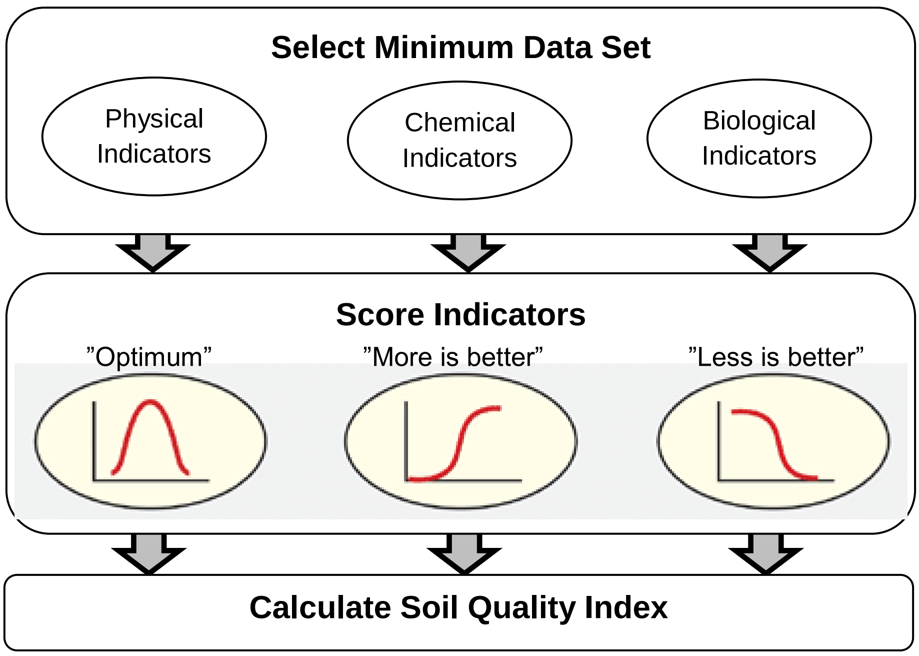


Figure 3.2 Conceptual model for converting minimum data set indicators to soil quality index (after Karlen et al., 2003).

The sub-scores are suggested to be integrated using the arithmetic mean (Andrews et al., 2004):

$$I_j = \frac{1}{n}\sum_{i=1}^{n} s_{ji} \, , \tag{3.2}$$

where I_j is soil quality index for j-th remediation alternative, s_{ji} is the sub-score of i-th soil quality indicator and n is the number of indicators.

3.3 Uncertainty analysis

Monte Carlo simulation

Monte Carlo simulation is a technique for calculating uncertainties in the model results by including uncertainties in input variables. This technique is used in the work presented in Papers II-IV to account for the uncertainties in soil classification.

Using a large number of trials, uncertainties in the model results are calculated by randomly sampling values from the probability distributions for each uncertain variable in the model (Figure 3.3).

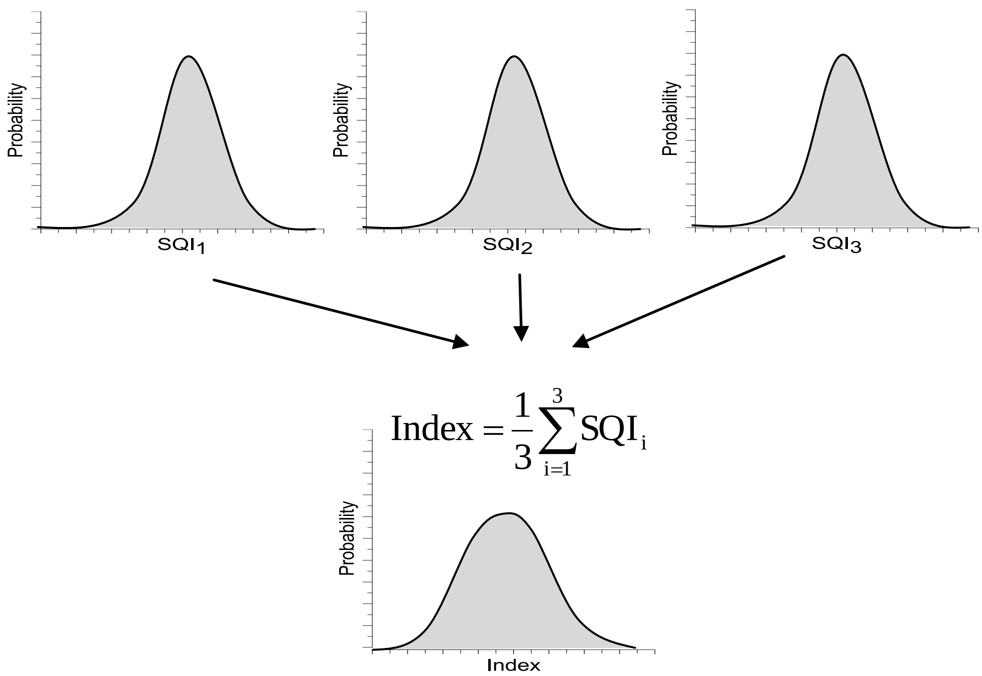


Figure 3.3 Illustration of how Monte Carlo simulations can be used to include uncertainties in input variables (SQI_i) and the result (Index).

Mathematical description of Monte Carlo simulation methods is provided in Bedford and Cooke (2001) and Press et al. (1995). A brief description of the properties of the most frequently used probability distributions in Monte Carlo simulations is provided in Taylor (1997).

4 RESULTS AND APPLICATIONS

In this chapter the results in terms of the developed approach to evaluation of soil functions and services within a generic MCDA for sustainability assessment of remediation alternatives, the developed method for soil function assessment and the case study applications are described.

4.1 Hierarchy between soil functions and soil ecosystem services

The first step in achieving the aim of the study was to provide the terminology used throughout the work. For definitions the reader is referred to Papers I and IV. Sometimes the terms relevant to the soil functions, the soil quality and the ecosystem services concepts are used interchangeably. To avoid confusion, the distinctions between key terms used in the sol function concept are outlined with help of relevant questions in Table 4.1.

Table 4.1 The selected terms relevant to the soil function, the soil quality and the ecosystem services concepts (modified from Carter, 2002).

KEY TERMS	RELEVANT QUESTIONS
Purpose of the soil	What is the soil used for?
Soil ecosystem service	What are the benefits humans gain from the soil use?
Soil function	What is the role of the soil in the ecosystem?
Soil process	What are the biotic and abiotic interactions supporting the function?
Soil property	What are the critical soil attributes for maintenance of the soil process?
Soil quality indicator	What is a threshold value of the measurable soil attribute for maintenance of the soil process?

Further, the terminology compiled in Paper I suggests a hierarchy between functions, processes and services provided by an ecosystem (including a soil ecosystem). As the aim of a sustainability assessment of remediation alternatives is to evaluate whether a remediation alternative contributes to sustainable development or not, it was also important to link the suggested hierarchy to the three domains of sustainability. An hourglass model was therefore suggested to better describe the above mentioned linkages and the hierarchy (Figure 4.1).

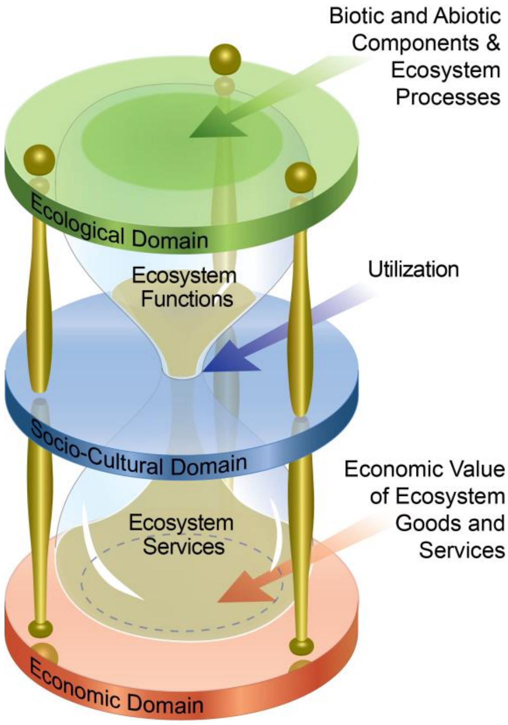


Figure 4.1 The hourglass of sustainability (Volchko et al., 2013).

Although the term "ecological domain" is used in Figure 4.1, "environmental domain" is consistently used throughout the thesis to reflect not only ecology but also ecosystems' capabilities to absorb wastes and provide natural resources for humans. In the environmental domain the ecosystem processes are based on the ecosystem structure and interactions between its biotic and abiotic components. These processes result in ecosystem functions. Ecosystem functions turn into ecosystem services once they are used by humans and thus pass into the socio-cultural domain. When an ecosystem service has an economic value, this service is transferred to the economic domain (Figure 4.1).

Utilization is a bottleneck in the hourglass model (Figure 4.1). Like grains of sands run faster through a wider hourglass neck, so are natural resources quicker depleted through overuse. Since some ecosystems' components and processes are unique and irreversible over relevant time horizons, the quick depletion of natural resources affects the potential of ecosystems to provide services critical for present and future generations. The limits of utilization are usually defined on the political level by developing and adapting a variety of regulatory requirements and environmental laws, e.g. the proposed EU Soil Framework Directive (COM, 2006) for sustainable use of soil resources.

4.2 Generic approach to soil function assessment

The suggested generic approach to evaluation of soil functions and services within an MCDA for sustainability assessment of remediation alternatives is presented in Paper I. The effects on the soil performance are suggested to be measured using SQIs and soil service indicators (Figure 4.2).

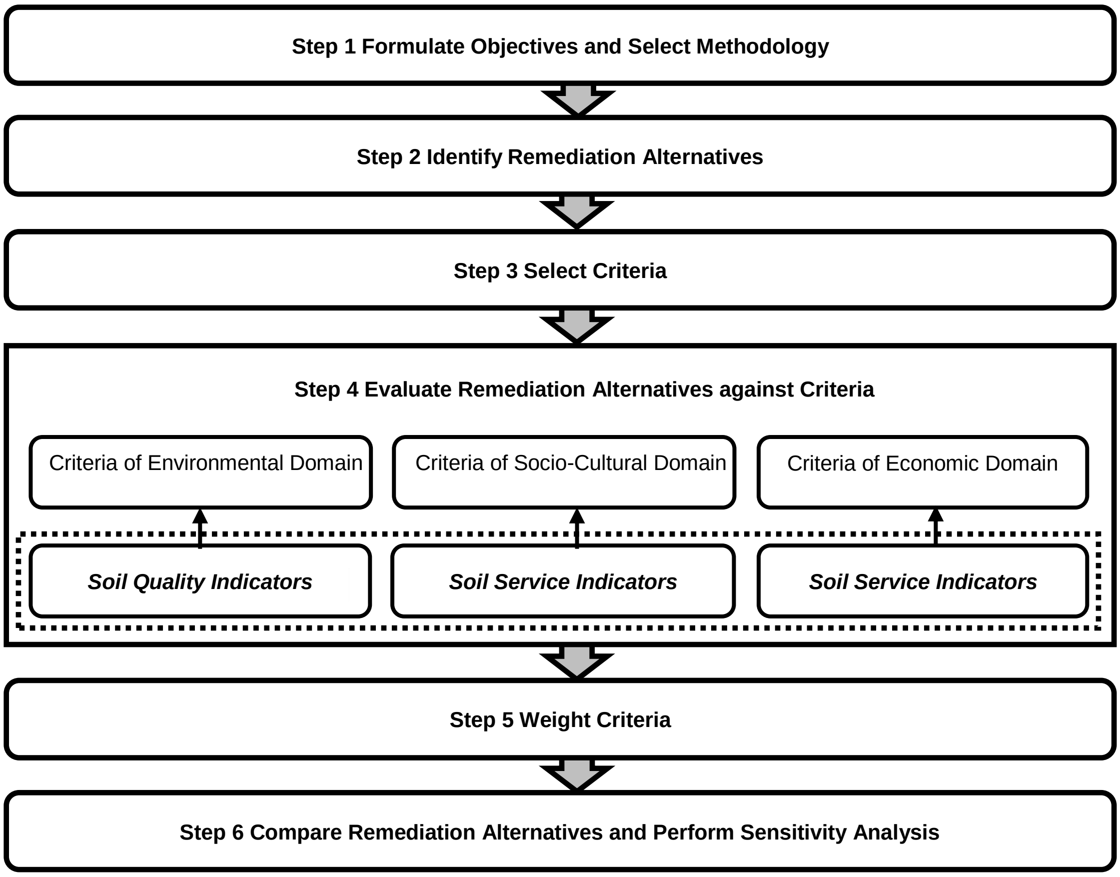


Figure 4.2 *Incorporation of the soil function concept into an MCDA framework for sustainability assessment in soil remediation projects (Volchko et al., 2013). The grey arrows indicate the main flow of assessment. The black arrows and the dotted box correspond to soil function evaluation.*

The effects of remediation alternatives on ecological soil functions should logically be evaluated in the environmental domain of the sustainability assessment of remediation alternatives using SQIs (Figure 4.2). In accordance with the above outlined hierarchy between soil functions and soil ecosystem services, these functions are what the soil system does in its natural state. Using the hierarchy as a selection criterion and based on Table 2.1, the main ecological soil functions were summarized in Table 4.2.

Table 4.2 The main ecological functions of the soil.

ECOLOGICAL SOIL FUNCTIONS
Basis for primary production
Basis for biodiversity
Habitat for flora and fauna
Biogeochemical cycling (e.g. water, carbon, nitrogen, phosphorus cycles)
Biological population control and disease suppression
Soil formation
Soil structure maintenance
Filtering and buffering of toxic compounds
Resistance and resilience of the soil system

Notably, the first three soil functions outlined in Table 4.2 are supported by the other six. In the proposed EU Soil Framework Directive the ecological functions are (*i*) storing, filtering and transforming nutrients, substances and water; and (*ii*) biodiversity pool, such as habitats, species and genes. Further, (*iii*) biomass production including agriculture and forestry can be considered as reflecting both an ecological soil function (e.g. basis for primary production) and a soil ecosystem service (e.g. provision of food, fiber and timber).

Non-ecological functions of the soil are "functions for people" and related to socio-economic effects of remediation alternatives. Given an ecosystem services perspective, social and economic soil functions, e.g. (*iv*) physical and cultural environment for humans and human activities; (*v*) source of raw materials; (*vi*) acting as carbon pool; and (*vii*) archive of geological and archeological heritage as included in the proposed EU Soil Framework Directive, can be categorized as soil ecosystem services, as opposed to ecological soil functions. Once ecological or non-ecological soil functions are utilized by humans for the benefit, they immediately turn into soil ecosystem services (see Figure 4.1). The effects of remediation alternatives on soil ecosystem services should be evaluated in the socio-cultural and the economic domains of the sustainability assessment using soil service indicators (Figure 4.2). These indicators are value-related measurements that indicate to which degree a management action contributes to human well-being by preserving, restoring and/or enhancing a soil ecosystem service. The value-related measurements can be expressed in: (1) community-based values which reflect attitudes, preferences, and intentions associated with a soil service; (2) economic values revealed by market data (if any) about a soil service, or the willingness to pay (WTP) for the service provided by the end use of the soil (SAB, 2009).

4.3 Development of soil function assessment method

This section describes the developed method for soil function assessment in the environmental domain of the MCDA using SQIs. The method consists of six steps (Figure 4.3).

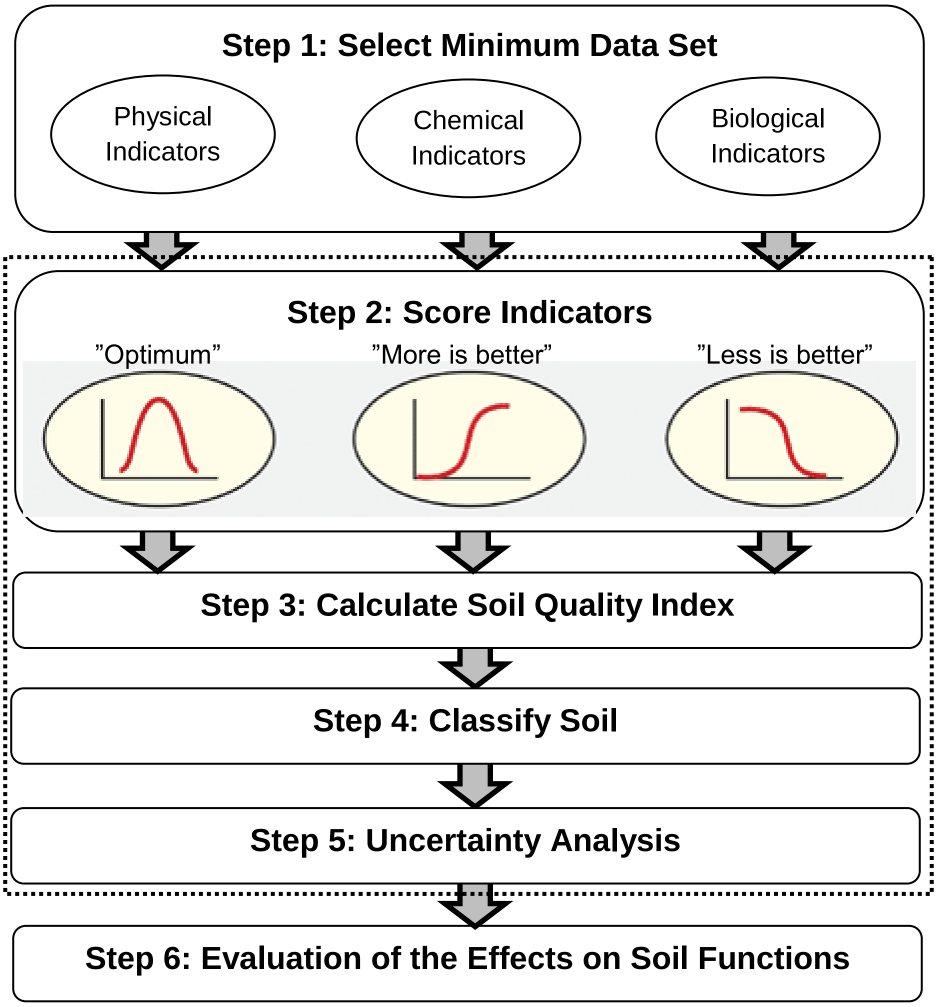


Figure 4.3 *A suggested method for evaluation of the effects of remediation alternatives on soil functions (modified after Karlen et al., 2003).*

These are : (1) selection of a minimum data set; (2) scoring of soil quality indicators; (3) calculation of soil quality index; (4) soil classification, (5) uncertainty analysis of the obtained results and (6) evaluation of the effects on soil functions. Application of the method on case studies is presented in Papers II-IV. Each step of the suggested soil function assessment method is described in detail below.

Step 1: Identification of minimum data set

Assessment of different soil functions requires different sets of SQIs. The MDS for soil functions associated with primary production was derived based on literature (Paper II). The suggested MDS includes seven physical, chemical and biological soil quality indicators (Table 4.3).

Table 4.3 The suggested MDS for assessment of ecological soil functions in remediation projects. SQI: soil quality indicator. ST: soil texture. CM: content of coarse material. AW: available water capacity. OM: organic matter content. NH_4-N: potentially mineralizable N. P: available phosphorus.

SQI	RELEVANCE TO SOIL FUNCTIONS
ST	Water infiltration, plant-available water and nutrient retention, aeration, root penetration.[1] Adsorption of heavy metals, the capacity of the soil to bind contaminants and thus protect from contamination.[2]
CM	The increased content of coarse particles (>2 mm) and presence of debris affect soil aggregate stability (i.e. ability to withstand falling apart when wet or hit by raindrops) as well as prevent plant rooting, decrease plant-available water and decline organic matter levels.[1]
AW	Cycling of water in the soil. Water between the field capacity and the wilting point is the crucial factor of storing water in the soil for soil organisms between precipitations.[1]
OM	Cycling of carbon in the soil. Presence of organic matter leads to (1) improvement of soil aggregate stability, water storage potential, nutrient cycling, and (2) increased microbial diversity/ activity and thus increased carbon sequestration.[1]
NH_4-N	Cycling of nitrogen in the soil. Ability of microbial communities to supply plant-available nitrogen, a measure of biological activity.[1]
pH	The indicator revealing the level of toxicity and nutrient availability.[1] Reflecting a potential for filtering and buffering of heavy metals.[2]
P	Phosphorus cycling. Macronutrient for plants and a measure of soil fertility.[1]

[1]Gugino et al. (2009), Idowu et al. (2008) and Schindelbeck et al. (2008). [2]Lehmann et al. (2008).

Step 2: Scoring of soil quality indicators

Using a custom fit option of the Grapher Golden software v.8.0.278, scoring functions were derived using least square methods to approximate the relevant data provided in the literature (Table 4.4). This data reflects the relationships between sub-scores and the measured SQIs. The sub-score interval for a soil of poor soil quality is 0 – 0.3, for medium soil quality is 0.31 – 0.7, and for good soil quality is 0.71 – 1. Three types of scoring curves were developed for soil function assessment: “more is better”, “optimum”, and “less is better” (Papers II-III).

Table 4.4 *Sources of data for determination of scoring functions. ST: soil texture. BD: bulk density. CM: content of coarse material. OM: organic matter content. AW: available water capacity. NH4-N: potentially mineralizable N. P: available phosphorus.*

SUB-SCORES	ANALYSIS METHOD	SCORING FUNCTION TYPE	SOURCE OF DATA/COMMENT
CM	Sieving (ISO 3310-2:1999)	“Less is better”	The threshold value (i.e. a sub-score of 0.3) for soil functions associated with primary production is a content of coarse material equal to 35%. The coarse fraction content less than 15% is scored higher than 0.7 (Craul and Craul 2006).
AW	Determination of pore volume contents of soils based on ST, OM and BD (Lehmann et al., 2008)	“More is better”	Gugino et al. (2009)
OM	Loss on ignition (SS-EN 12879:2000)	“More is better”	Gugino et al. (2009)
NH_4-N	Anaerobic incubation (Gugino et al., 2009)	“More is better”	Gugino et al. (2009)
	Distillation (APHA, 1992)		The scoring function is based on the estimated representative values provided by a certified laboratory.
pH	pH (H_2O) (ISO 10390:2005)	“Optimum”	The scoring curves for vegetation favoring neutral and acidic pH are based on data provided by Gugino et al. (2009) and Swedish EPA (1999) respectively.
P	Morgan-P (McIntosh, 1969)	“Optimum”	Gugino et al. (2009)
	Olsen-P (ISO 11263:1994) AL-P (SS 02 8310:1993)		The scoring function follows the same shape as that for Morgan-P. The agronomic optimum values of Olsen-P (15.2-26.4 mg/kg) and AL-P

Total P (SS-EN ISO 11885-1)	(92.3-107 mg/kg) are provided by Osztoics et al., (2011). The agronomic values of Total P (411-450 mg P kg^{-1}) are provided by Pautler and Sims (2000).

Step 3: Calculation of soil quality index

Thereafter, for integrating information from soil quality indicators into the management decision process, all sub-scores are integrated into a soil quality index using the arithmetic mean of the sub-scores (Eq. 3.2), or the geometric mean

$$I_j = \sqrt[n]{\prod_{i=1}^{n} s_{ji}} \,, \tag{4.1}$$

where I_j is soil quality index for j-th remediation alternative, s_{ji} is the sub-score of i-th soil quality indicator and n is the number of indicators. The main difference between the aggregation methods is that, in contrast to the arithmetic mean, the geometric mean does not allow for compensation of a strong performance on one SQI by a weaker performance on another one. If at least one SQI performs poorly generating a low sub-score, the soil quality index generated by geometric mean of the sub-scores will also result in a low value.

Step 4: Soil classification

The soil quality index forms a basis for soil classification into five soil classes corresponding to *very good*, *good*, *medium*, *poor* and *very poor soil performances* (Table 4.5).

Table 4.5 Correspondence between soil classes, soil performances and a soil quality index (modified after Gugino et al, 2009; Volchko et al., 2014).

SOIL CLASS	PERFORMANCE	INDEX
1	Very good	> 0,85
2	Good	0,70 – 0,85
3	Medium	0,55 – 0,69
4	Poor	0,40 – 0,54
5	Very poor	< 0,40

Step 5: Uncertainty analysis

The uncertainties in the resulting indices and soil classes are handled with Monte Carlo simulations. Assuming that all SQIs are normally distributed and accounting for sample size, translated and scaled *t*-distributions are used to represent the uncertainties of the mean value of each SQI. The parameters of the *t*-distribution are the mean value of the SQI, the scale ($\frac{s}{\sqrt{n}}$), and the degrees of freedom ($n-1$), where s is the standard deviation and n is the number of soil samples (Gelman et al. 2004). The normality assumption is based on analysis of data from three studied sites: Hexion, Kvillebäcken and Marieberg (description of the cases is provided below).

Step 6: Evaluation of the effects on soil functions

The effects of remediation alternatives on soil functions are addressed in the soil functions sub-criterion in the environmental domain of SCORE. Using the matrix of effects (Figure 4.4), the effects are evaluated relative to a soil class in a reference alternative following the 21-grade scores as suggested by the SCORE method: Very positive effect: +6 to +10; Positive effect: +1 to +5; No effect: 0; Negative effect: -1 to -5; Very negative effect: -6 to -10. The reference alternative is usually a base case scenario, where no remedial action is taken.

Soil class of reference alternative	Soil Class as a result of remediation alternative				
	1*	**2***	**3***	**4***	**5***
1	0	-4	-8	-8	-8
2	+4	0	-4	-8	-8
3	+8	+4	0	-4	-8
4	+8	+8	+4	0	-4
5	+8	+8	+8	+4	0

Soil Quality Classes:

1	Very good
2	Good
3	Medium
4	Poor
5	Very poor

Effects on Soil Functions:

+6 to +10	Very positive
+1 to +5	Positive
0	No effect
-1 to -5	Negative
-6 to -10	Very negative

Figure 4.4 The suggested matrix for scoring the effects on soil functions as an input to the MCDA framework (modified after Volchko et al., 2014). The example marked by arrows in the figure shows a case where the soil in the reference alternative is classified as soil class 3 and where the soil after remediation is predicted to become soil class 2, the effect thus being positive (+4).

Since the scoring is associated with uncertainties, probability distributions for the scores are assigned instead of point values, in accordance with a three step procedure in SCORE (see Section 3.1).

4.4 The SF Box tool

Since the effects of remediation alternatives in SCORE for sustainability assessment are evaluated relative to the reference alternative, it is important to evaluate ecological soil functions for a base case scenario. Based on the method outlined in Section 4.3, the SF Box tool was developed to assist evaluation of ecological soil functions for the reference alternative. The assessment steps carried out in the tool are indicated with dotted box in Figure 4.3. The overall input/output flow in SF Box is presented in Figure 4.5.

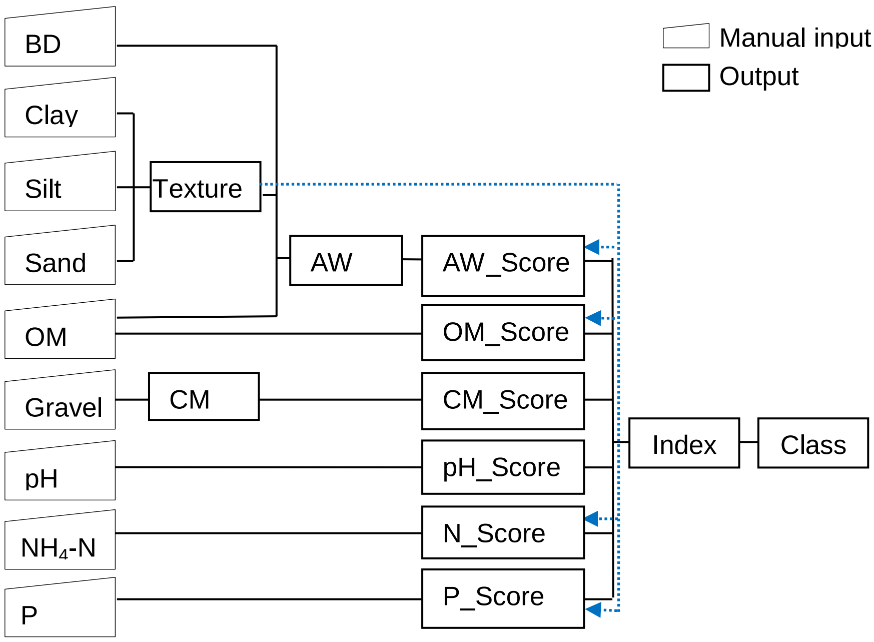


Figure 4.5 The overall input/output flow in SF Box. BD –bulk density, OM – organic matter content, NH_4-N – potentially mineralizable N, CM – content of coarse material, AW – available water capacity, P – available phosphorus. AW_Score, OM_Score, CM_Score, pH_Score, N_Score, P_Score – the computed scores for available water capacity, organic matter content, content of coarse material, pH, potentially mineralizable N and available phosphorus respectively.

Available water capacity is computed as a function of soil texture, bulk density and organic matter based on the pore volume estimations of mineral soils (Lehmann et al., 2008). The bulk density is not a part of the MDS, however, the likeliest value of this SQI should be selected from the dropdown menu of the program in order to compute available water capacity. Content of coarse material equals to the gravel content in the soil sample. Soil texture is computed as a function of the percentages of clay, silt and sand contents in the soil sample using the Food and Agriculture of United Nations (FAO) soil texture triangle (Lehmann et al., 2008). Further, the scores reflecting the performance of each indicator are computed for all indicators from the suggested MDS except for soil texture (Table 4.3). The soil texture is not scored directly, but is used to score potentially mineralizable N, organic matter content, available water capacity and available phosphorus. Further, the soil quality index and the corresponding soil class are computed for integrating information from SQIs into a management decision process.

In order to address the soil functions sub-criterion of the soil criterion in SCORE, the last step (Figure 4.3), i.e. scoring of the effects of remediation alternatives on soil functions, is carried by assessor using the soil class calculated by SF Box (Figure 4.5) and the suggested matrix for scoring the effects on soil functions (Figure 4.4).

4.5 Case studies

The soil functions were assessed for four study sites: Hexion, Kvillebäcken, Marieberg and Riksten. The first two are urban sites situated in Mölndal and Gothenburg respectively. Soil function assessment results for these sites are presented in Paper III. The last two are rural sites situated in the municipalities of Kramfors and Botkyrka respectively. Soil function assessment results for the Marieberg site are presented in Paper IV.

All study sites are former industrial areas heavily contaminated with various compounds (Table 4.6). For all sites except Riksten investigations were carried out and human health and ecological risk assessments were performed. The risks posed to human health and the environment are found to be unacceptable at all investigated sites (Sweco, 2009, 2010; Fanger et al., 2007).

Table 4.6 Contaminants, former activities at and location of the study sites.

CASE STUDY	CONTAMINANTS	ACTIVITY	LOCATION
Hexion	Lead, aliphatic hydrocarbons, DEHP, PAHs	Paint factory	City of Mölndal
Kvillebäcken	Lead, copper, aliphatic and aromatic hydrocarbons, PAHs	Small industries including paint production	City of Gothenburg
Marieberg	PCDD/Fs	Saw mill	Kramfors municipality
Riksten	PAHs	Coal/ pine tar industry	Botkyrka municipality

For the Hexion and the Marieberg sites sustainability assessments of remediation alternatives were performed including assessment of the effects on soil functions (the full sustainability assessment for Hexion is presented in Paper V). The Kvillebäcken and the Riksten sites were used as complementary case studies for soil function assessment.

Hexion

The Hexion site is located in Mölndal, south of Gothenburg, the western part of Sweden. Hexion is a former industrial site, with a former paint factory producing chemicals and binding agents (Figure 4.6). The industrial activities lasted from the 1940s until 2007. After remediation, the site is planned to be used for apartment blocks, school and preschool, shops and offices, traffic areas and parking lots and green areas with playing grounds.

Hexion is situated in the Gothenburg terminal moraine deposit. The soil deposits have a complex composition with varying fraction distribution, from well-sorted sand and gravel to glacial till with lenses of finer grains. The depth of the soil is generally 5-15 meter with glacial till closest to the bedrock, followed upwards by sand, gravel and silt (for details see Landström and Östlund, 2011). As a result of the long history of industrial activity there are large amounts of filling materials on top of the natural deposits. The filling material mostly consists of sand, gravel, bricks and asphalt (NCC Teknik, 2010).

The ground water flows 2-10 m below the surface in a north-south direction. The groundwater is artesian forming a spring in the steep slope of the Hexion site. The ground water connects to the river Mölndalsån, which runs south-east of the site. High flows and the erosional environment in the river beds prevent accumulation of contaminants in the sediments near the site. The risk posed by the contaminants at the site to the receptors in the River Mölndalsån is considered to be low (Sweco, 2009).

Figure 4.6 *Aerial photo over Trädgården 1:124, Hexion. The white line marks the border of the site and the dotted line marks Mölndalsån (Landström and Östlund, 2011). Photo: National Land Survey of Sweden, Gävle, Sweden. © Lantmäteriet i2012/1099*

There are parts of the area where the earlier activities have caused substantial contamination of both soil and groundwater, primarily by phthalates, lead and solvents. The contaminants are mostly found in the upper soil layers (0-1 m) but within limited parts of the area, high concentrations of specific contaminants have been found at greater depths.

Exposure pathways for humans with the future land use (as described above) are in the form of oral intake of contaminated soil, direct skin contact with contaminated soil, and inhalation of dust originating from contaminated soil. The site-specific risk assessment shows that exposure to volatile contaminants beneath the new buildings is not regarded to be an issue because the constructions will be sealed preventing volatiles from entering the buildings. There is a need to reduce the human health risks, and the risks posed to the environment.

Four remediation alternatives are considered in this study:

Alt A. To excavate all soil with a concentration of contaminants above the generic guideline values as issued by the Swedish EPA, and to transport the soil by trucks to a suitable landfill (Heljestorp, Kikås, Skara).

Alt B. To excavate all soil with a concentration of contaminants above the site-specific guideline values. The soil is transported by trucks to suitable landfills (Heljestorp, Kikås, Skara).

Alt C. To excavate all soil with a concentration of contaminants above the site-specific guideline values. The excavated soil is sieved at the site, the coarse fraction is reused at the site and the finer fractions are transported by trucks to suitable landfills (Heljestorp, Kikås, Skara).

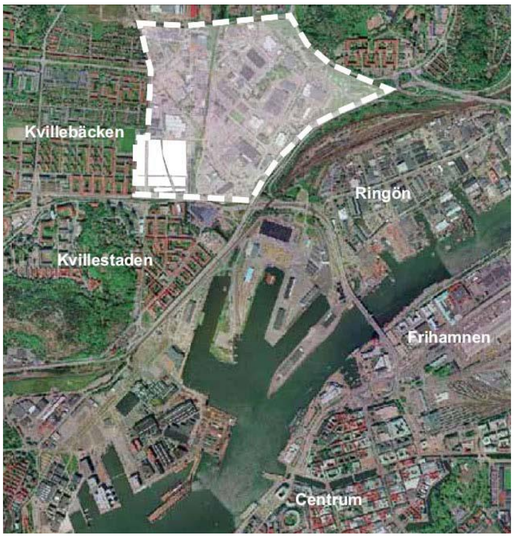
Alt D. To excavate all soil with a concentration of contaminants above the site-specific guideline values. The excavated soil is sieved and washed at the site, the coarse fraction is reused at the site and the finer fractions are transported by trucks to suitable landfills (Heljestorp, Kikås, Skara).

Kvillebäcken

The Kvillebäcken site is situated in Gothenburg, south-west Sweden. It is a former industrial site with small industries and other related activities. The site has been divided into 21 lots that have been allocated to a total of 7 lot owners. Eastern Kvillebäcken, which is a part of the redevelopment of a larger area, will primarily be developed into a residential area, with multi-family dwellings and such elements as retail premises, kindergartens, club rooms and the like (Figure 4.7). One part of the redevelopment area, in the vicinity of the residential area, is going to be turned into a green area. This area is located along the Kvillebäcken stream.

The superficial soil layers in the Kvillebäcken area consists of filling material with a variable thickness, over 2 m in Eastern Kvillebäcken and about 0.3- 0.5 m in the western part. Beneath the filling material is glacial marine clay with a thickness of about 30-40 m, which is situated directly on crystalline gneissic rock, sometimes with a thin layer of glacial till between the clay and the rock. Groundwater appears in the lower part of the filling material, on top of the sealing clay, or in the dry clay crust, and in the rock beneath the clay deposits. The general groundwater flow direction in the superficial layers is east towards the

Kvillebäcken stream. Locally, pipes and pipe trenches greatly affect the flow direction.



(a)

(b)

Figure 4.7 *a) Eastern Kvillebäcken indicated with a filled rectangle inside of the whole redevelopment area (indicated with dotted line); b) Illustrated detailed plan for Eastern Kvillebäcken (the park area is the area on the eastern part of Eastern Kvillebäcken). Source: GS (2008).*

Several environmental soil investigations have been carried out in the area. The studies show that soil is contaminated by past activities to a varying degree. High to very high concentrations of metals, aliphatic and aromatic hydrocarbons and PAHs have been detected in soil samples. Groundwater samplings show that despite high levels of pollutants in the soil, generally no contaminants, metals or organic substances, are found in the groundwater. The effects of pollutants on soil layers from previous activities primarily concern the filling material, although the underlying clay in occasional points has also been impacted in superficial parts in some locations.

Leaching tests for metals for the Kvillebäcken site have been performed on a collection of samples representing different filling materials. The concentrations at different ratios between liquid and solid material (L/S) were compared to the Swedish EPA's criteria for waste disposal. The concentrations of all investigated parameters are below the criteria for inert waste, with an exception for the fluoride content, which is slightly higher than the corresponding threshold (NCC Teknik, 2000).

Marieberg

The former Marieberg sawmill site is situated in northern Sweden, Kramfors municipality. The site situated along the Ångermanälven river and covers an area of approximately 1500 m x 150 m. Chlorophenol (CP) based wood preservatives was used for more than two decades until closure of the sawmill activities in 1970. The CP preservatives were contaminated with polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs, commonly called 'dioxins'). These compounds are toxic and highly persistent organic pollutants, and the site is still heavily polluted (Åberg et al. 2010). The site includes former saw mill and impregnation (the hot spot) (A), resident house (B), former wood storage (C), former drying house (D), pastures and farm (E), culture area with resident houses and hostel (F), former timber yard (G), cutter shaving tip and present-day camping (H), village (I) (Figure 4.8).

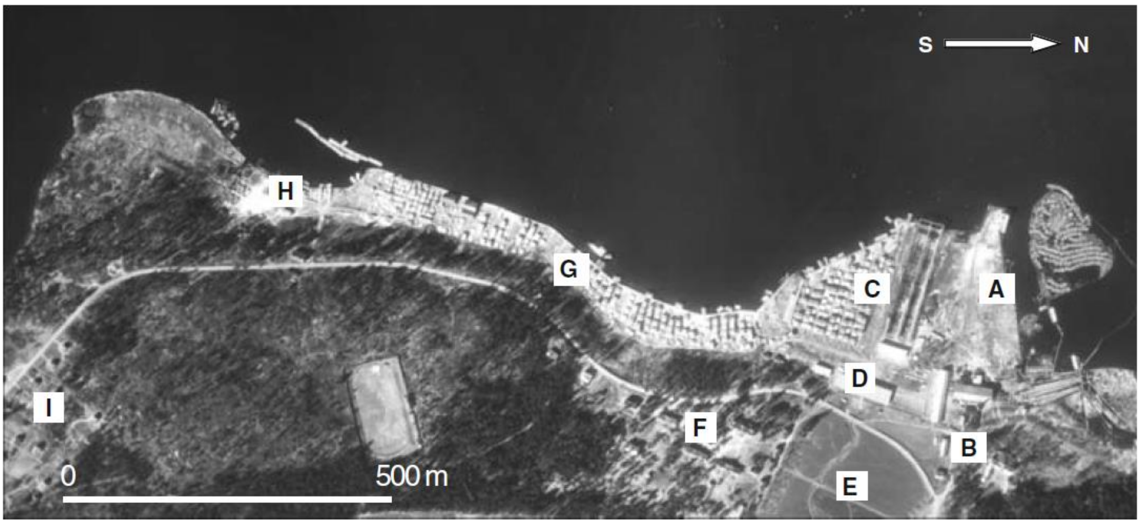


Figure 4.8 *Aerial photo over the industrial area during its active period (1862–1970) (Åberg et al. 2010). Photo: National Land Survey of Sweden, Gävle, Sweden.* © Lantmäteriet i2012/1099

Most of the area consists of filling material (0-4 m). Fillings consist mainly of silt mixed with sand, gravel and / or clay and in some places mixed or layered with cortex and sawdust (Fanger et al., 2007). Wood and brick occurs sporadically in the fillings, as well as concrete and similar waste materials. Loose sediment deposits mostly consisting of sulphide silt and sulphide clay underline the filling material. The thickness of sediment deposits increases from east to west towards the river. Glacial till is found along the river bank at depths of 10-15 m. The site also has three landfills – a wood chip/sawdust dump and the lower and upper industrial landfill. The lower industrial landfill consists of industrial and municipal wastes. A large part of the landfill includes cortex and ash but also scrap metal, hardboard, cable and brick. Various filling materials were found in the upper industrial landfill such as sand, silt, clay, cortex, wood chips, bricks and elements of scrap.

The site is in the process of being remediated, and based on the alternatives suggested for the site, three remediation alternatives are considered within this study:

Alt A. Excavation of masses with a concentration of contaminants above generic guideline values. The alternative assumes replacement of the contaminated soil with a clean soil.

Alt B. Excavation of hot spots. The alternative assumes replacement of the heavily contaminated soil in the hot spots with a clean soil. This alternative has been discussed by the authorities but was in the specific case not chosen mainly due to concerns connected with future land use.

Alt C. Environmental risk area – conservation of the site. The alternative prohibits access to the area by fences and assumes no remedial action. This alternative is a part of the presented research project only. However, the alternative is possible within current legislation and is therefore of interest, especially concerning the effects on soil functions and the socio-cultural domain.

Riksten

The site of the former Riksten coal/pine tar factory is about 0.5 ha and situated in Botkyrka municipality, in the western part of Sweden. Riksten is located in a sediment deposit consisting of fine sand (MIFO, 2012). The site is today covered by forest-like vegetation. The Bysjön lake is situated to the west of the site. Residential houses are situated in a close proximity of the site (in 50-100m).

The Riksten site is classified as an area with risk class 1 (a very high risk to human health and the environment) according to the MIFO method (in Swedish: Metodik för Inventering av Förorenade Områden) for inventory of contaminated areas (MIFO, 2012). Residual products of coal/pine tar industry are coal tar, pine tar and pitch, i.e. liquids of high viscosity and are complex mixtures of phenols and PAHs. Some places of the site are covered with coal tar. Petroleum odor is detected in the area. A number of tanks and barrels with a creosol-similar liquid were observed at the site. It is suspected that the soil is severely contaminated with PAHs, creosols and heavy metals as a result of earlier activities and is now posing risks to human health and the environment. Contaminants may spread from the soil to groundwater and surface water in the nearby lake.

Soil sampling

At the Hexion and the Kvillebäcken sites the soil was sampled to two depths 0 - 0.2 m and 0.2 - 0.5 m using a shovel. For each site 16 soil samples in total were collected for analysis of SQIs from the suggested MDS. The soil at Hexion was sampled randomly within "green" area of the site (Figure 4.6). The soil at the west bank of the stream within the future park area at Kvillebäcken was sampled along a line parallel to the stream with an approximate sample separation of 25m to a depth of 0.2 m (Figure 4.7 b).

At Marieberg (areas indicated with A, C and D in Figure 4.8) and Riksten the soil was sampled randomly to a depth of 0.5 m using an excavator. In total 18 and 10 soil samples respectively were collected. For analysis of SQIs from the MDS, ten increments were collected from different parts of each excavated soil pile, placed in bucket and well homogenized to ensure representativeness of the soil sample. Thereafter, the remaining material in each soil pile was sieved through a 2 mm mesh in the field and well homogenized in order to analyze contaminant concentrations. Before analysis of organic matter, potentially mineralizable N, the NH_4-N concentration, pH and available phosphorus, the soil samples from all sites were sieved through a 2 mm mesh at the laboratory.

Soil analysis

The particle size distribution analyses for Marieberg, Riksten, and Kvillebecken were performed at the Agrilab laboratory (Uppsala) by the soil sieving method, after the soil was oven-burned at 550°C (ISO 3310-2). The particle size distribution analysis of the soil samples from Hexion was performed at the WSP laboratory (Gothenburg) using the same method. For Hexion and Kvillebäcken, phosphorus was extracted with ammonium lactate and quantified by inductively coupled plasma (ICP) spectrometry at the laboratory at the Swedish University of Agricultural Sciences (SLU, Uppsala) (AL-P, Egner et al., 1960 and SS 02 8310). Using the same method for analysis of phosphorus, the soil samples from Marieberg and Riksten were analyzed at the Alcontrol laboratory.

Total C and total N for Riksten and Marieberg were analyzed at the ALS Scandinavia laboratory (Luleå) by dry combustion in a Leco analyzer. Using the same method for analysis of total C and N, the soil samples from Kvillebäcken (0.2-0.5m) and Hexion were analyzed at the Agrilab laboratory (Uppsala) and from Kvillebäcken (0-0.2m) at the laboratory at SLU. Before analysis for total C and total N, the soil samples from Kvillebäcken and Hexion were stored at 4°C for more than three months. For Hexion, Kvillebäcken, Marieberg and Riksten, potentially mineralizable N was analyzed at the Agrilab laboratory (Uppsala) with a one week anaerobic incubation under saturated conditions at 30°C (Gugino et al., 2009). Before analysis of potentially mineralizable N, the soil samples were stored at 4°C for more than three months.

All other SQIs for four study sites were analyzed at the Alcontol laboratory (Linköping). The NH_4-N concentration was analyzed by distilling the sample with a sodium hydroxide solution prior to titration with hydrochloric acid (Mulvaney, 1996; APHA, 1992). The organic matter content was determined at as a loss on ignition at 550°C (SS-EN 12879). pH was determined using a glass electrode in a 1:5 (volume fraction) suspension of soil in water (ISO 10390). The available water capacity was indirectly determined by using the relationship between the FAO (Food and Agriculture Organization of the United Nations) soil texture class, organic matter content and bulk density as described by Lehmann et al. (2008), assuming a bulk density of 1.6 g cm^{-3}.

For the Marieberg and the Riksten sites, contaminant concentrations were quantified at SLU. The analyses of the concentrations of the seventeen 2,3,7,8-substituted CDD/Fs and the sixteen PAHs were performed using gas chromatography coupled with high resolution mass spectrometry (GC-HRMS) at the Environmental Chemistry Laboratory, Umeå University, which is accredited for this type of analysis. The isotope dilution method, with isotopically labelled standards for all congeners, was used for quantification.

Soil function assessment

According to the FAO texture triangle, the soils at the Hexion and the Marieberg sites were classified as sands and loamy sands. At the Kvillebäcken site the soils were classified as silty and sandy loams. At the Riksten site the soils varied from silty loams to sands. Basic statistics for the analyzed SQIs from the MDS for the study sites is presented in Table 4.7.

Table 4.7 Basic statistics for the analyzed SQIs from the MDS at the studied sites.

	CM, [%]		AW, [%]		OM, [%]		NH4-N, [mg/kg]		pH		AL-P, [mg/kg]	
	1	2	1	2	1	2	1	2	1	2	1	2
HEXION												
m	15	18	22	22	2.8	3.3	183	172	6.1	6.4	95	106
Std	11	10	1.2	1.5	1.9	2.6	22	30	0.4	0.4	59	67
Min	4	5	21	21	0.8	0.9	160	120	5.6	5.7	21	29
Max	37	34	24	25	5.7	8.9	220	210	6.7	6.8	197	230
CV	0.7	0.5	0.1	0.1	0.7	0.8	0.1	0.2	0.1	0.1	0.6	0.6
KVILLEBÄCKEN												
m	8	32	25	24	8.1	8.3	248	241	5.8	5.9	59	53
Std	4	19	2.7	0.7	4.3	5.8	96	96	0.6	0.6	38	38
Min	3	13	20	23	2.6	4.1	180	170	5.1	4.9	9	9
Max	17	55	28	25	16.8	22.2	470	440	6.5	6.6	134	101
CV	0.5	0.6	0.1	0.1	0.5	0.7	0.4	0.4	0.1	0.1	0.6	0.7

	CM, [%]	AW, [%]	OM, [%]	NH4-N, [mg/kg]	pH	AL-P, [mg/kg]
MARIEBERG						
m	13	22	2.8	190	6.6	34
Std	6.5	1.5	2.2	25	0.7	10
Min	2	21	0.6	140	5.6	20
Max	21	25	7	230	8.2	59
CV	0.5	0.1	0.8	0.1	0.1	0.3
RIKSTEN						
m	25	25	26.7	505	5.6	131
Std	17	2.3	20.4	225	0.6	66
Min	10	21	7.4	200	4.7	56
Max	55	28	76.5	900	6.6	270
CV	0.7	0.1	0.8	0.4	0.1	0.5

1: depth of 0-0.2m. 2: depth of 0.2-0.5m. *m*: mean. Std: standard deviation. Max: maximum. Min: minimum. CV: coefficient of variation. CM: content of coarse material (ø>2 mm). AW: available water capacity. OM: organic matter content. NH_4-N: ammonium concentration determined with a distillation method. AL-P: available phosphorus.

Other SQIs were also analyzed to inform on N mineralization and the degree of contamination at the site (Table 4.8). For Kvillebäcken and Riksten, potentially mineralizable N was determined as a difference between the NH_4-N concentrations before and after anaerobic incubation of a soil sample. For all the sites this SQI was also predicted using a first order exponential function (Stanford and Smith, 1972):

$$N_t = N_0\left(1 - e^{-kt}\right), \tag{5.1}$$

where N_t is the cumulative N mineralized at week *t*, N_0 is the soil N pool, *k* is the miniralization constant ($k = 0.054wk^{-1}$), and *t* is time in weeks. It was assumed that the soil N pool (N_0) equals to 1-5% of total N in the soil (Springob and Kirchmann, 2003).

Table 4.8 Basic statistics for the additional SQIs.

	Total N, [%]		NH4-N*, [µg/g per wk]		NH4-N**, [µg/g per wk]	C:N		
HEXION								
	1	2	1	2	-	1	2	
m	0.07	0.09	1.8	2.3	-	58	39	
Std	0.06	0.07	1.7	1.9	-	44	31	
Min	0.01	0.01	0.3	0.3	-	16	18	
Max	0.14	0.2	3.7	5.3	-	111	89	
CV	0.9	0.8	0.9	0.8	-	0.8	0.8	
KVILLEBÄCKEN								
	1	2	1	2	1	1	2	
m	0.24	0.26	6.4	6.8	9.3	20	22	
Std	0.16	0.26	4.1	6.8	10.6	10	11	
Min	0.5	0.06	1.3	1.6	1	14	12	
Max	0.58	0.86	15.2	22.6	29.4	38	39	
CV	0.6	1	0.6	1	1.1	0.5	0.5	
MARIEBERG								
	Total N, [%]		NH4-N*, [µg/g per wk]		NH4-N**, [µg/g per wk]	C:N		Sum PCDD/F 17, [pg/g]
m	0.16		3.8		-	6		31 000
Std	0.05		1.2		-	5		46 000
Min	0.1		2.6		-	1		210
Max	0.26		6.8		-	19		160 000
CV	0.3		0.3		-	0.8		1.6
RIKSTEN								
	Total N, [%]		NH4-N*, [µg/g per wk]		NH4-N**, [µg/g per wk]	C:N		Sum PAH 16, [mg/kg]
m	0.27		18		25	21		44
Std	0.32		8.5		15.8	8		79
Min	0.27		7.1		1	12		1.3
Max	1.3		34.2		46	37		260
CV	0.5		0.5		0.6	0.4		1.8

1: depth of 0-0.2m. 2: depth of 0.2-0.5m. m: mean. Std: standard deviation. Max: maximum. Min: minimum. CV: coefficient of variation. NH4-N*: potentially mineralizable N determined as a function of total N. NH4-N**: potentially mineralizable N determined with one week anaerobic incubation.

The C:N ratio was reported to inform on quality of organic matter at the studied sites. The N content of soil organic matter as reflected through the C:N ratio, is of primary importance in regulating magnitude of organic matter mineralization and immobilization. The optimum C:N ratios for mineralization of OM in arable soils are 10-15 (Springob and Kirchmann, 2003). The mean C:N ratios at Hexion, Kvillebäcken and Marieberg are not optimal for N mineralization (Table 4.8). It should be noted that ratios are prone to considerable variations resulting from errors in determining both variables (total C and total N). Ratios of C:N smaller than 2 and higher than 70 should be considered as outliers (Batjes, 1996). The optimal C:N ratios for forest soils differ from arable soils and range between 25 and 30 (Lukac and Godbold, 2011). A C:N ratio < 25 may lead to nitrate leaching in forest ecosystems. At the Riksten site with forest-like vegetation and acidic soils, the mean C:N ratio is < 25 (Table 4.8).

Contaminant concentrations were reported for the Marieberg and the Riksten sites to inform on the degree of contamination at the sites. The contaminant concentrations had a high variability in contrast to other SQIs (Table 4.7; Table 4.8). Linear dependencies between the organic matter content and the PCDD/F and PAH concentrations were observed. Coefficients of determination, R^2=0.37 and R^2=0.81, in the regression models for Marieberg and Riksten respectively indicated that 37% of variability in PCDD/F concentration and 81% of variability in PAH concentration could be explained by the linear relationship with organic matter content. The Pearson's population correlation coefficients were computed to be R = 0.61 and R = 0.89 for Marieberg and Riksten respectively. A strong correlation between surface soil organic matter and organic pollutants has been reported in other studies (e.g. Bergknut et al., 2010; Meijer et al., 2002; Meijer et al., 2003).

For all four studied sites strong linear relationships were observed between total C, total N, OM and NH_4-N determined with the distillation method (Table 4.9). For Riksten a linear dependency between NH_4-N (determined with the distillation method) and potentially mineralizable N (determined with the incubation method) was observed (R=0.73). Coefficient of determination (R^2= 0.54) in the regression model indicated that 54% of variability in potentially mineralizable N could be explained by the linear relationship with NH_4-N.

Table 4.9 *Matrix of correlation coefficients for the Hexion, the Kvillebäcken, the Marieberg and the Riksten sites.*

	Total C	Total N	C:N	NH4-N	OM
			HEXION		
Total C	1				
Total N	0.99	1			
C:N	-0.93	-0.96	1		
NH_4-N	0.74	0.73	-0.83	1	
OM	0.79	0.78	-0.85	0.95	1
			KVILLEBÄCKEN		
Total C	1				
Total N	0.84	1			
C:N	-0.01	-0.45	1		
NH_4-N	0.72	0.95	-0.40	1	
OM	0.94	0.96	-0.30	0.86	1
			MARIEBERG		
Total C	1				
Total N	0.77	1			
C:N	0.98	0.67	1		
NH_4-N	0.67	0.65	0.59	1	
OM	0.96	0.87	0.92	0.70	1
			RIKSTEN		
Total C	1				
Total N	0.95	1			
C:N	0.95	0.88	1		
NH_4-N	0.93	0.99	0.87	1	
OM	0.99	0.95	0.93	0.92	1

OM: organic matter content.

NH_4-N: ammonium concentration determined with the distillation method.

Using the SF Box tool, the ecological soil functions associated with primary production were evaluated for the reference alternatives at the four sites (Table 4.10).

Table 4.10 Scoring results for the soil quality indicators of the suggested MDS for the Hexion, the Kvillebäcken, the Marieberg and the Riksten sites.

SOIL QUALITY INDICATOR	CASE STUDY											
	Hexion				Kvillebäcken				Marieberg		Riksten	
	0-0.2m		0.2-0.5m		0-0.2m		0.2-0.5m		0-0.5m		0-0.5m	
	1	2	1	2	1	2	1	2	1	2	1	2
CM	0.84	G	0.78	G	0.22	P	0.32	M	0.88	G	0.32	M
AW	0.90	G	0.90	G	0.95	G	0.93	G	0.91	G	0.95	G
OM	0.41	M	0.54	M	1	G	1	G	0.40	M	1	G
NH_4-N	0.01	P	0.01	P	0.20	P	0.08	P	0.02	P	1	G
NH_4-N*	0	P	0	P	0.07	P	0.09	P	0	P	1	G
NH_4-N**	-	-	-	-	0.44	M	-	-	-	-	1	G
pH	0.91	G	1	G	0.46	M	0.55	M	1	G	0.96	G
AL-P	0.95	G	0.8	G	0.92	G	0.88	G	0.55	M	0.35	M

1: score. 2: interpretation. G: good. M: medium. P: poor.
NH_4-N: Scoring for the NH_4-N concentration determined with a distillation method.
NH_4-N*: Scoring for potentially mineralizable N determined as a function of total N.
NH_4-N**: Scoring for potentially mineralizable N determined with the incubation method.
See also description of the abbreviations in Table 4.7.

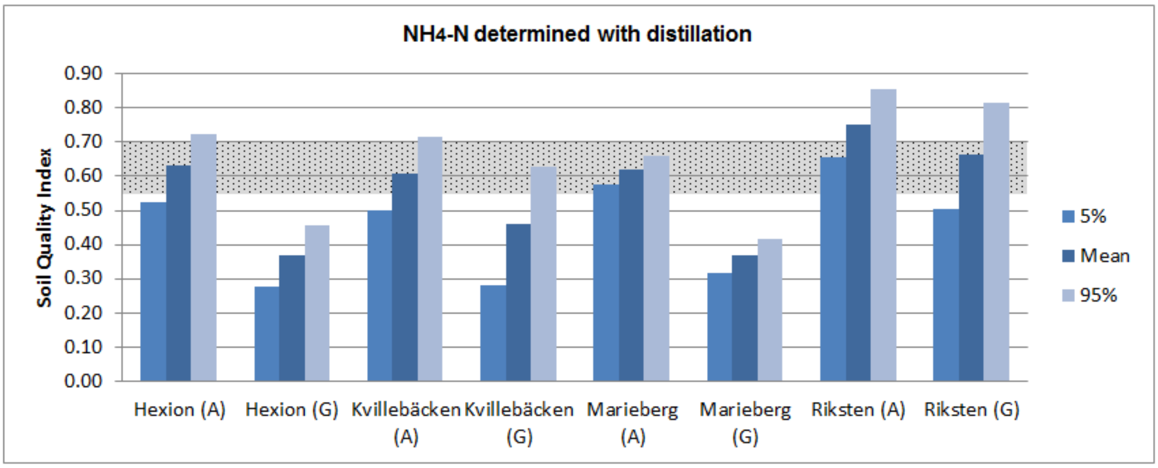
Two different scoring functions were used to score NH_4-N. One function was used to score the NH_4-N concentration determined with the distillation method. Another function was used to score potentially mineralizable N determined with anaerobic incubation (NH_4-N*) and as a function of total N (NH_4-N**).

The low sub-scores for NH_4-N at the Hexion, the Kvillebäcken and the Marieberg sites indicated the limited amount of plant-available N. The low sub-scores for the content of coarse fragments (ø>2mm) in the top layer at Kvillebäcken indicated plant rooting limitations. The high sub-scores for organic matter content at Kvillebäcken and Riksten indicated that the soil was rich in organic matter thus having a good potential for water storage and nutrient cycling. The sub-scores for organic matter at Hexion and Marieberg corresponded to medium soil quality. The high sub-scores for available water capacity indicated that the soils at the three sites were capable to store a sufficient amount of water in the soil for soil organisms between precipitations.

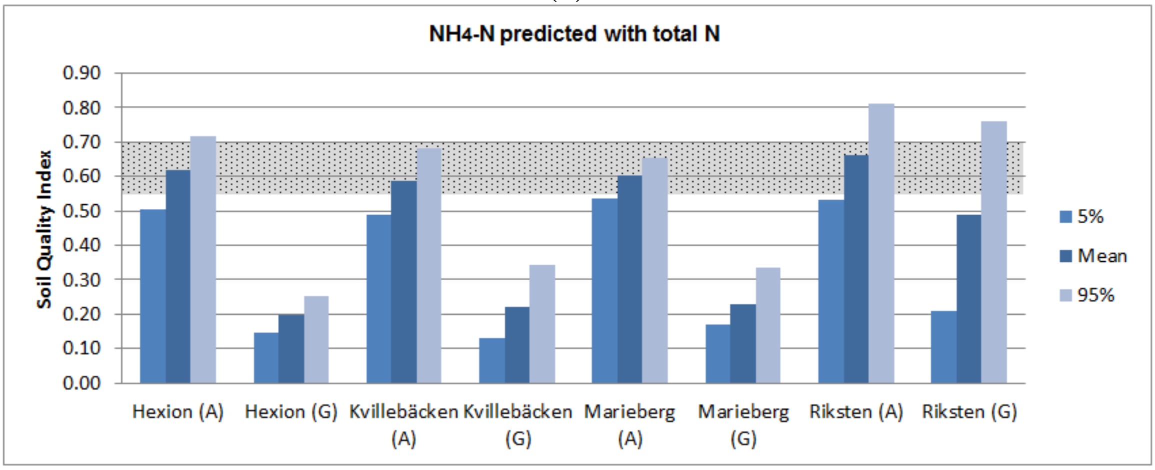
Although the soil at Riksten is heavily contaminated with PAHs, the soil function assessment results show that it has a good soil functioning potential.

The parameter uncertainties in SF Box were handled with Monte Carlo simulations using the Oracle Crystal Ball© software. Translated and scaled *t*-distributions were used to represent the uncertainties of the mean value of each SQI. Since bulk density is represented by five discrete values ranging between 1 to 1.8 g/cm^3 in accordance with the table for determination of the pore volume of mineral soils (Lehmann 2008), a discrete custom probability distribution is used to represent the uncertainty in this SQI. Uncertainties associated with the predicted potentially mineralizable N were handled by assigning *t*-distribution to the total N values and a beta distribution to the predicted percentage of mineralization to find a soil N pool (using minimum=0, maximum=100%, 5-th percentile=1% and 95-th percentile=5%).

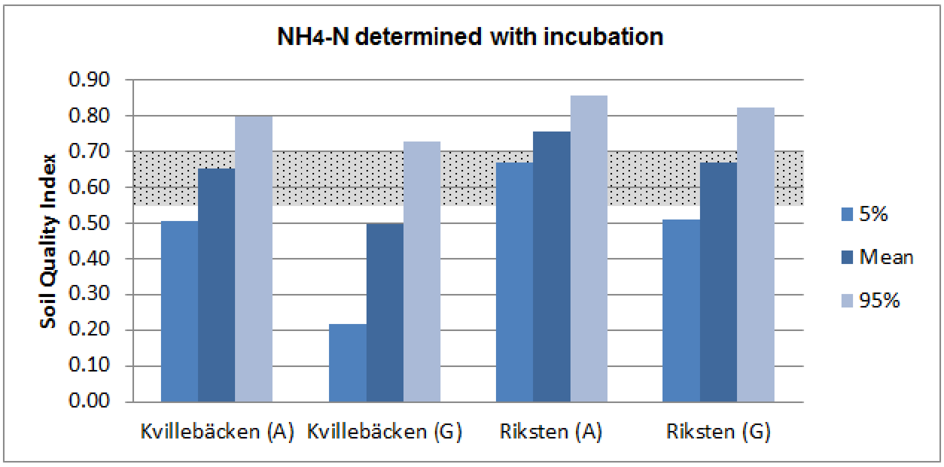
The mean, the 5- and 95-percentiles of simulated soil quality indices for the soils at the Hexion, the Kvillebäcken, the Marieberg and the Riksten sites are presented in Figure 4.9. Different results were generated depending on the method used for aggregation of the sub-scores and the method used for determination of NH_4-N. When the sub-scores were aggregated as arithmetic mean, for the Hexion and the Marieberg sites the simulated mean of the soil quality index corresponded to class 3 (medium soil performance) regardless the method for NH_4-N determination (Figure 4.9 a, b). The same was observed for the Kvillebäcken site (Figure 4.9 a, b, c). For Riksten the simulated mean of the soil quality index corresponded to class 2 (good soil performance) when the sub-scores were aggregated as arithmetic mean, and distillation and incubation were used for determination of NH_4-N (Figure 4.9 a, c). When NH_4-N was predicted with total N, the simulated mean of the soil quality index for Riksten corresponded to soil class 3 (medium soil performance). When the sub-scores were integrated as geometric mean, the simulated mean of the soil quality index for all sites except Riksten was lower than the limit separating the soils which are capable of performing its functions from those which are not (Figure 4.9 a, c). The aggregation method for the sub-scores affected the results of soil classification. The method for determination of NH_4-N had a slight impact on the soil function assessment results. However, the lower soil quality index was computed for the Riksten site when potentially mineralizable N was predicted as a function of total N (Figure 4.9 b).



(a)



(b)



(c)

Figure 4.9 *Histograms showing the mean, the 5- and the 95-persentales of simulated soil quality index for the soils at Hexion, Kvillebäcken, Marieberg and Riksten. The arithmetic (A) mean and the geometric (G) mean were used to aggregate the sub-scores. The dotted area corresponds to a medium soil performance.*

The last step of the soil function assessment as outlined in Figure 4.3 is carried out in SCORE for sustainability assessment. The effects of remediation alternatives on soil functions are scored relative to the soil class computed for the reference alternative using the matrix of the effects (Figure 4.4). The remediation alternatives at the Hexion site considered in this study assumed excavation and differed only in pre-treatment of the excavated material before disposal. Since special soil quality requirements should be fulfilled for installation works within green areas in accordance with AMA (2010), a refilling soil is assumed to be of class 2 (good soil performance). A change from class 3 (medium soil performance) in the reference alternative to class 2 as a result of remediation generates a positive effect on soil functions within future green areas of the remediation site.

For the Marieberg site, in the reference alternative, the soil corresponded to soil class 3 and a medium soil performance, when the sub-scores were aggregated as arithmetic mean (Figure 4.9). The effects of remediation alternatives on soil functions were evaluated relative to the reference alternative using a suggested matrix of the effects (Figure 4.4). The remediation alternative conservation of the site as "environmental risk area" will generate no effect, i.e. a score of 0. Depending on the soil class of the refilling material, the alternatives excavation and excavation of hot spots will generate different effects on soil functions and accordingly different scores (Table 4.11). Excavation of the hot spots and refilling with a clean material will not result in soil class 1 and 5 as an average over the entire area.

Table 4.11 Possible scoring of the effects on soil performance after remediation at the Marieberg site as a function of the refilling material.

REMEDIATION ALTERNATIVES	SOIL CLASS OF REFILLING MATERIAL				
	1	2	3	4	5
	”Very good”	”Good”	”Medium”	“Poor”	”Very poor”
Excavation	+8	+4	0	-4	-8
Excavation of Hot Spots	-	+2	0	-2	-

+8: very positive effect. +4: positive effect. 0: no effect. -4: negative effect. -8: very negative effect.

Obviously, the quality of the refilling material becomes a crucial factor for the future soil functioning.

5 DISCUSSION

In this chapter the contents of the thesis are discussed.

5.1 Functions vs. services

The suggested hierarchy between soil functions and soil ecosystem services formed a basis for incorporating the soil function concept (as included in the proposed EU Soil Framework Directive; COM, 2006; Table 2.1) into sustainability assessment of remediation alternatives. Soil functions are natural capabilities of the soil ecosystem, whereas soil ecosystem services are benefits humans gain from the soil ecosystem (i.e. utilized soil functions to yield human well-being). Some soil functions and soil ecosystem services, which are outlined in the proposed EU Soil Framework Directive, are considered in the SCORE framework. Soil functions covered in SCORE are (*i*) biomass production (i.e. basis for primary production in SF Box), and (*ii*) storing, filtering and transforming nutrients and water (i.e. cycling of water, carbon, nitrogen and phosphorus in SF Box). It is suggested to account for cultural soil ecosystem services, such as geological and archaeological archive, in the cultural heritage criterion of the socio-cultural domain of SCORE. Such provisioning (market-priced) soil ecosystem service as source of raw materials is suggested to be taken into account in the social profitability criterion of the economic domain of SCORE.

Soil functions are assessed in the environmental domain of sustainability using soil quality indicators, e.g. organic matter content and pH. Soil ecosystem services are suggested to be assessed in the socio-cultural and the economic domains of sustainability using value-related indicators, e.g. opinions, attitudes, WTP, and prices for ecosystem goods. In contrast, in the recent study by SuRF-UK (2011) ecosystem functions, goods and services are suggested to be evaluated in the environmental domain. However, as evident from the definitions of ecosystem services usually used in ecological economics, the goods and services resulting from soil functions might be more relevant to socio-economic effects of remediation.

5.2 Minimum data set

In this study the MDS for soil function assessment was derived using a screening method searching for the most frequently suggested SQIs in remediation projects and for non-agricultural purposes. A more advanced method of identification of SQIs would involve soil scientists into a screening process. The suggested MDS is relevant to soil functions associated with primary production and consists of soil texture, content of coarse material, available water capacity, organic matter content, potentially mineralizable N, pH and available phosphorus. It is generally recognized that an MDS should fulfil the following criteria: 1) sensitivity to variations in soil management; 2) good correlation with beneficial soil functions; 3) helpfulness in revealing ecosystem processes; 4) comprehensibility and utility for land managers; and 5) inexpensive and easy to measure (Doran and Zeiss 2000; Kruse 2007). The majority of the suggested MDS indicators (*i*) correlate well with soil functions associated with primary production (as shown by statistical analysis results in Gugino et al., 2009); (*ii*) reveal soil processes, e.g. N mineralization; (*iii*) are comprehensible for land managers (interpretation in terms of soil functions is available in the literature); and (*iv*) relatively inexpensive and easy to measure (tested at four sites in Sweden).

There is no general consensus on an MDS for soil function assessment in the literature. Thus, any MDS may be a topic of debate. Some MDS indicators can correlate well with a soil function but be interrelated. For example, available water capacity and organic matter in the suggested MDS correlate, because in the developed SF Box tool the former is determined as a function of the latter, bulk density and soil texture. Further, SQIs can have different threshold values which vary with a soil depth and the end use of the soil. For example, organic matter in the top layer is of great importance but less so in the subsoil, with typically a content of <1% in natural subsoil (Craul and Craul, 2006). A threshold pH value for a forest soil would be different from a threshold pH value for a grass field soil.

Different MDSs are demanded for assessment of different soil functions. Furthermore, the assessment results may be interpreted differently for different soil functions (Table 5.1). Also, the same SQI can be interpreted differently for different management goals, e.g. ‘‘more is better’’ for NO_3-N supporting plant growth but ‘‘less is better’’ with regard to protection of the environment from nitrate leaching (Karlen et al., 2003). The majority of SQIs are function-dependent. However, the suggested MDS captures multiple soil functions associated with primary production, i.e. water, carbon, nitrogen and phosphorus cycling in the soil. The cross-functional MDSs relevant to primary production were also suggested by Gugino et al. (2009), Idowu et al. (2008), and Schindelbeck et al. (2008).

Table 5.1 Correspondence between soil functions and soil classes for the examined samples of a stagnic luvisol soil (Lehmann et al., 2008).

SOIL FUNCTION	SOIL CLASS	SOIL QUALITY
Basis for Life and Habitat of flora and fauna	5	Very poor
Component of the Water Cycle	4	Poor
Component of the Nutrient Cycle	1	Very good
Filter and Buffer of Heavy Metals	2	Good
Transformation Medium	4	Poor

Potentially mineralizable N

Potentially mineralizable N determined with the anaerobic incubation method is listed as an important biological indicator of soil quality (Doran and Parkin, 1994; Stenberg, 1997; Schomberg et al., 2009). This SQI was used by several authors for comparison with more rapid methods for determination of N mineralization (for review see Ros et al., 2011). For the Riksten site potentially mineralizable N strongly correlated with NH_4-N determined with the distillation method. Strong correlations between these SQIs were also reported in the previous studies (Sharifi et al., 2007; Bushong et al., 2008). The NH_4-N concentration determined with the distillation method can therefore be used as a proxy of biological activity for N in the soil. Furthermore, potentially mineralizable N can be determined indirectly using a first order exponential function (Stanford and Smith, 1972) and assuming that the soil N pool equals to 1-5% of total N (Springob and Kirchmann, 2003). The developed scoring functions for potentially mineralizable N and the NH_4-N concentration determined with the distillation method generated slightly different sub-scores, which corresponded to the same sub-score intervals representing a poor soil quality for Hexion, Kvillebäcken and Marieberg, and a good soil quality for Riksten (Table 4.10).

The C:N ratio can complement the suggested MDS by informing on the magnitude of organic matter mineralization and immobilization. To better inform on biological activity in the soil, potentially mineralizable N can be complimented with basal respiration, substrate-induced respiration (SIR) or metabolic quotient, qCO_2 (respiration to microbial biomass ratio). Stenberg (1997) recommended to include both N mineralization and SIR into a MDS for integrated evaluation of physical, chemical and biological properties of the soil.

It should be noted that storage of soil samples can significantly impact the analysis results. The biological properties are not affected when soil samples are stored at 4°C for up to three months and at -20°C for up to one year (Stenberg et al., 1997). In this study, before analysis of potentially mineralizable N, the soil samples were stored at 4°C for a longer period, which could affect the analysis results. For the Marieberg and the Hexion sites, the analysis results for this SQI were lower than the detection level. For the Kvillebäcken site, no correlation were observed between potentially mineralizable N and organic matter (OM), although these SQIs are usually strongly correlated (Gugino et al., 2009). Still, strong correlations were observed between NH_4-N determined with a distillation method, OM, total N and total C for all case studies (Table 4.9).

5.3 Soil function assessment method

In remediation projects, the information from SQIs can be integrated into a decision-making process using the suggested soil function assessment method. This method is performed by (i) transformation of the measured SQIs into sub-scores, i.e. fractional numbers in the interval [0; 1]; (ii) aggregation of the sub-scores into a soil quality index using one of three available aggregation methods (Section 4.3); and (iii) soil classification into one of five classes (Table 4.5). The transformation is done (a) to normalize input SQIs, i.e. bringing the data from different scales (e.g. percentages and mg/kg) into one scale – fractional numbers in the interval [0; 1], and (b) to interpret the SQIs in the context of soil functions. For example, a content of coarse material of 36% corresponds to a sub-score of 0.28, i.e. “poor soil quality”, preventing plant rooting, decreasing plant-available water, and declining organic matter levels.

The developed soil function assessment method is associated with a number of limitations. The method is only relevant for the upper ~0.5 m of the soil within future green areas of remediation sites. The scoring functions for the available water capacity, the organic matter content, potentially mineralizable N and pH were derived from the statistical models developed for vegetable and crop production systems (Gugino et al., 2009). Furthermore, the data used for modelling is collected across the North-eastern United States. Thresholds for American and Swedish soils may differ. The scoring function for available phosphorus was developed based on the agronomic optimum values and thresholds reflecting phosphorus leaching to the environment (Osztoics et al., 2011; Pautler and Sims, 2000). The soil quality requirements for agricultural land and green areas of remediation sites may also differ. For example, nutrient cycling and supply requirements are much different for crop production sites with intensive farming than for forest ecosystems and urban land uses (Karlen et al., 1997). Admittedly, interpretation of the measured SQIs should be done in the context of the land use objectives. However, interpretation of SQIs for urban land uses is scarce in the literature.

Further, in the developed scoring models the highest scores are assigned to the measured SQI values reflecting the full potential of the “ideal” soil to carry out its functions associated with primary production. In this study, the “ideal” soil is represented by a coarse fraction content of <15%, an available water capacity of >18%, an organic matter content of >4.8%, potentially mineralizable N of >11μgN/g dry matter per week, pH ranges of 4.4-5.8 and 6-7.5 for vegetation favoring acidic and neutral soils respectively, available phosphorus of 92-107 mg AL-P/kg. However, in reality the full potential may differ for different types of soils. For example, for some soils, 2% total organic carbon (TOC) would receive the highest score whereas for other soil types, 2% TOC would represent a degraded soil and would be scored accordingly. Therefore, advanced soil function assessment requires involvement of soil experts in remediation projects.

The developed soil function assessment method is operationalized to offer practitioners in remediation a tool. The tool allows for transformation of input SQIs into sub-scores further integrating them into a soil quality index which corresponds to one of five soil classes. Although the arithmetic mean is suggested for aggregation of the sub-scores (Andrews et al. 2004; Gugino et al., 2009), the SF Box tool provides the possibility to use the geometric mean for calculating the soil quality index. As it was demonstrated in Figure 4.9, selection of the method for aggregation of the sub-scores can have a large impact on the assessment results. Uncertainties in the resulting soil quality index and soil classification are treated by Monte Carlo simulation in the SF Box tool. However, the add-in Oracle Crystal Ball software is required for running simulations. Although the suggested method for soil function assessment is generalized and somewhat simplified, it can provide practitioners with comprehensible information on basic soil properties with regard to soil functions relevant to the green areas of remediation sites as a complement to ecological risk assessment.

5.4 Decision support

Being critical for ecosystem survival and human well-being, soil functions form an important aspect of sustainability assessment of remediation alternatives, especially when the goal of remediation is to protect the soil environment. The developed soil function assessment method is operationalized with help of SF Box and integrated into SCORE for sustainability assessment in remediation projects. The information from SQIs provides a land manager with input on the soil functions sub-criterion in SCORE and allows for an assessment of the impact of remediation alternatives on selected ecological soil functions.

A soil quality index generated with help of SF Box provides information on the soil's ability to carry out its functions associated with primary production, whereas contaminant concentration is related to the risks posed to the soil organisms. It is therefore suggested to treat ecotoxicological risks and soil functions in two different sub-criterions of the soil criterion in SCORE. Results of correlation analysis for the Marieberg and the Riksten studies support such division. Although a positive linear correlation was observed between contaminant concentrations and the organic matter content for these study sites, no linear relationships were observed between the contaminant concentrations and the soil quality index. Contaminant concentrations and a soil quality index thus provide different types of information that complement each other.

As the effects of contaminants in the field may differ from predictions with SSD models, it is important to account not only for contaminant concentrations but also for bioavailability of contaminants, their toxicity and ecological effects on a biota as suggested by the Triad approach to ecological risk assessment (Swartjes et al., 2012b). In addition, other soil conditions that enables the soil biota to operate should be considered in remediation projects. For example, availability of water and nutrients is critical for soil organisms. The effects of the remedial action itself on the soil environment should be accounted for in a soil management process. The suggested MDS for soil function assessment may be used to ensure preservation/re-establishment of favorable conditions in the soil for vegetation as a result of the remedial action, accounting for a coarse fraction content, available water, organic matter, pH, a plant-available form of N and available phosphorus.

The case studies suggest that soil contamination does not necessarily mean poor soil functions. Neither does it necessarily mean that reduction of risks posed by contaminants to the environment results in restoration of soil functions. Although the soil at Riksten is heavily contaminated it has a good potential to carry out its functions associated with primary production (Figure 4.9). For the Marieberg site, the effects of remediation alternatives on soil functions strongly depend on the quality of the refilling material (Table 4.11). Therefore, the soil functions can be depleted if soil quality is only maintained with regard to contaminant concentrations ignoring physical, biological and other chemical soil properties.

In order to ensure restoration of ecological soil functions after remediation, special care needs to be taken with respect to physical, chemical and biological properties of the soil material in the upper ~0.5 m where active life takes place. A well-structured soil profile should be built/preserved as a result of remedial action in order to provide favorable conditions for primary production within future green areas. Such a profile consists of three basic layers: (*i*) the top layer of 15-20 cm, which is rich in organic matter, (*ii*) the sub-layer of 50-60 cm serving as mechanical support and as a reservoir of nutrients and water, and (*iii*) the drainage layer of at least 15-20 cm, which is capable of transmitting excess water from the sub-layer (Craul and Craul, 2006). Admittedly, special soil quality requirements exist for green areas in the built environment (AMA, 2010). Before placement into a plant bed, the soil must be sampled and analyzed for soil texture, coarse fraction content, clay content, organic matter, salinity, pH, phosphorus, potassium and magnesium (AMA, 2010), i.e. SQIs rather similar to the suggested MDS. In addition, soil loosening is required to prevent compaction. For the Hexion and Kvillebäcken sites located in urban environments, it is therefore likely that replacement of the excavated contaminated soil of class 3 (medium soil performance) with a refilling material that fulfils the above mentioned soil quality requirements may lead to improvement of soil functions within future green areas. However, no soil quality requirements ensuring proper conditions for soil functioning exist for rural sites as e.g. Marieberg and Riksten.

Although the information from the suggested SQIs is intended to provide input to SCORE for sustainability assessment, it can also be used as basic information by practitioners for developing remediation strategies. For example, if the soil has potentially favorable conditions for providing ecological soil functions, alternative remediation strategies can be considered, e.g. reducing risks by immobilization of contaminants with soil amendment and also enriching the soil with nutrients, improving soil moisture retention, and stimulating biological activity in the soil (see also Cundy et al., 2013).

6 CONCLUSIONS AND FUTURE RESEARCH

In this final chapter the main conclusions are summarized and the future research aspects are outlined.

6.1 Conclusions

The following major conclusions were drawn from this work:

- Soil functions are natural capabilities of the soil ecosystem, whereas soil ecosystem services are benefits humans gain from the soil ecosystem (i.e. utilized soil functions to yield human well-being). The effects of remediation on soil functions can be assessed using physical, chemical and biological soil quality indicators. Soil ecosystem services are more related to socio-economic effects of remediation and can therefore be assessed using value-related indicators.

- The conceptualized hierarchy between soil functions and services, as well as the generic approach to soil function assessment can be applied in various land management projects using MCDA approaches to sustainability assessment of decision alternatives based on the three pillar model.

- The developed MDS consisting of soil texture, content of coarse material, available water capacity, organic matter, potentially mineralizable N, pH, and available phosphorus can be used for assessment of soil functions associated with primary production. The MDS may well further be developed in order to more stringently assess biological aspects of the soil which contribute to primary production. Another set of SQIs is required to assess e.g. biodiversity function.

- The developed scoring method for soil function assessment allows for interpretation of the measured SQIs and integration of this information into sustainability assessments of remediation alternatives. However, the threshold values used for scoring in this study were developed for the soils in the USA and therefore may differ from Swedish conditions.

- The same SQI can be analyzed using different methods which may provide different results. For example, the results for determination of mineralizable N with chemical and biological methods differ (Gianello and Bremner, 1986). Interpretation of the measured value requires development of a scoring curve relevant to a particular analytical method. It is also preferable to analyze soil samples for a particular SQI at the same laboratory to ensure comparability of the results.

- It is desirable that analysis methods for MDS indicators are standard methods. The anaerobic incubation method used in this study for determination of potentially mineralizable N is not common in Sweden. Instead, this indicator can be measured indirectly as a function of total N as the dry combustion method for analysis of total N is a standard method usually run in Sweden. Alternatively, the NH_4-N concentration determined with the distillation method can be used as a proxy of biological activity for N.

- Special care needs to be taken with regard to physical, chemical and biological soil properties of the upper soil layer at the remediation sites to ensure future proper soil functioning.

- Being a part of SCORE for sustainability assessment of remediation alternatives, the developed SF Box tool allows the practitioner to assess soil functions associated with primary production and to account for those aspects of soil quality which could otherwise be ignored. There is a potential for using SF Box for soil function assessment not only in remediation projects but also for other types of land management projects.

6.2 Future research

There are four priority aspects that are recommended to be considered in future research:

- Complementing the developed MDS with relevant biological soil quality indicators for assessment of soil functions associated with primary production;

- Development of MDSs for assessment of other soil functions, e.g. biodiversity;

- Adaptation of the developed scoring curves for soil function assessment to Swedish conditions;

- Calibration of the scoring curve for the NH_4-N concentration determined with the distillation method;

- Development of scoring curves for other soil quality indicators.

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