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ABSTRACT

The proposed EU Soil Framework Directive from 2006 has recognized soil functions as critical for ecosystem survival and human well-being. To meet emerging regulatory requirements on soil protection, this report presents an Excel-based tool, SF Box, for evaluating the effects on soil functions in remediation projects. The evaluation of ecological soil function is based on scoring of a set of soil quality indicators and computing a soil quality class for each remediation alternative. In order to evaluate the effects of remediation alternatives on soil functions, a soil quality class for each alternative is compared against the soil quality class in the reference alternative. By doing so, the SF Box tool provides a summary of the effects caused by remediation alternatives on soil functions, where the effects are scored between -2 representing "very negative effect" and +2 representing "very positive effect". A score of 0 represents "no effect". For demonstrating the basic possibilities of SF Box, the report includes examples on soil function evaluation in remediation projects.

Key words: Soil function, Brownfield (Contaminated sites), Soil quality indicator, Remediation, Sustainability

Contents

Preface

In this study, evaluation of the effects on soil functions in remediation projects is realized in the MS Excel using Visual Basics for Applications (VBA). The work is a part of two interrelated research projects on sustainability appraisal of remediation alternatives with focus on soil functions, ecosystem services and goods. The study is carried out at the competence centre FRIST and the Department of Civil and Environmental Engineering, Division of Geo Engineering, Chalmers University of Technology, Sweden. The projects are financed by the SNOWMAN ERA-Net and the Swedish Research Council Formas.

This part of the project has been carried out with Lic. Eng. Yevheniya Volchko as a researcher, Professor Lars Rosén as supervisor, Associate Professor Jenny Norrman and Ph.D. Malin Norin as co-supervisors. Associate Professor Tommy Norberg at the Department of Mathematical Sciences, Chalmers University of Technology & University of Gothenburg, Sweden is highly appreciated for advice.

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Yevheniya Volchko

1 Introduction

Soil functions are critical for ecosystem survival and human well-being, because only a healthy soil can enable the entire ecosystem to function properly. Being a subset of ecological processes, soil functions are a product of the "complex interactions between biotic (living organisms) and abiotic (chemical and physical) components of ecosystems [arising] through the universal driving forces of matter and energy" (de Groot, 2002). A great many of today's soil scientists denote an equal degree of importance to three soil quality elements comprising of the physical, the chemical and the biological soil properties (e.g. Andrews et al., 2004; Doran and Zeiss, 2000; Schindelbeck et al., 2008). Balanced and intense interconnections of these three soil quality elements are at the core of properly functioning soil.

Inherited from the era of industrialization, soil contamination unfortunately continues to be a widespread threat of soil functioning throughout the world. Striving for addressing the issue, the research in recent decades has resulted in a wide palette of available remediation techniques to address chemical soil quality, i.e. reduce contaminant concentrations and amounts in the soil to tolerable levels guided by intended land use (Swedish EPA, 2009). When evaluating sustainability of remediation alternatives, it becomes however important to consider the unity of three soil quality elements (composed of chemical, as well as physical and biological properties) for ensuring that the effects on soil functions are properly taken into account.

The best practice for sustainable remediation includes a framework for decision-making that considers pros and cons of available remediation alternatives usually using a Multi Criteria Decision Analysis (MCDA) (Rosén et al., 2009; CL:AIRE, 2011). The MCDA for sustainability appraisal of remediation alternatives provides a structure capturing a set of ecological, socio-cultural and economic criteria. However when several alternatives are available, soil function evaluation within sustainability appraisal can become a time- and effort-consuming task. For this reason, this report is aimed at presenting SF Box, a tool that has been developed to facilitate evaluation of the effects on soil function using a set of physical, chemical and biological soil quality indicators. The ultimate goal of the SF Box tool is to provide the input on soil functions for sustainability appraisal in remediation projects.
The report is structured as follows:
- A brief background to the study is summarized in Section 1.
- The overall input/output flow in the SF Box tool is presented in Section 2.
- An application example of SF Box is presented in Section 3.
- The uncertainties in the output results of SF Box are discussed in Section 4.
- Some concluding remarks are summarized in Section 5.

1.1 Background

The soil function concept and the MCDA prototype by Rosén et al. (2009) form two points of departure in this study. This section provides a brief description of these.

1.1.1 The soil function concept

Having an intensely interconnected and often interdependent relationship with ecosystems, soil functions have been recognized as critical for ecosystem survival and human well-being by scientific as well as political communities. Lehmann and Stahr (2010) provide a historical background of the soil function concept which originates from late 1970-ies when other soil functions than agricultural productivity of land were recognized by scientific communities (Table 1.2).

Table 1.2:   A historical background of the soil function concept (after Lehmann and Stahr, 2010).

Soil Functions	Sources
Buffer for energy, water, nutrients and pollutants	Schlichting (1972)
Securing food production Providing and cleaning ground water Filter, buffer and transformation of pollutants	Brümmer (1978)
Medium for plant growth and productivity Partitioning and regulating of water flow in the environment Environmental buffer	Larson and Pierce (1994)
Biomass production Reactor (filters, buffers, transforms matter) Biological habitat and genetic reserve	Blum and Santelises (1994)
Sustaining biological activity, diversity and productivity Regulating and partitioning water and solute flow Filtering buffering, degrading, immobilising, and detoxifying organic and inorganic materials Storing and cycling nutrients and other elements	Soil Science Society of America (1995)
Recycling organic materials to release nutrients and energy Partitioning rainfall at soil surface Maintaining stabile structure to resist water and wind erosion Buffering against rapid changes in temperature, moisture and chemical elements Storing and gradually releasing nutrients and water Partitioning energy at the soil surface	Warkentin (1995)
Biomass production, including in 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	European Commission (COM, 2006)

Once ecological, social or economic soil function is used by humans it is called an ecosystem service (e.g. de Groot, 2006). Admittedly, the soil can serve as (*i*) resource of biomass production for agricultural and forestry purposes, (*ii*) achieve of geological and archeological heritage; (*iii*) source of raw materials; (*iv*) carbon pool, (*v*) physical and cultural environment for humans and human activities (Table 1.2). However, these functions are of special meaning for individuals and a society as a whole, but are not vital for supporting life and habitat in ecosystems. These functions "for people" are more related to ecosystem services provided by soil resources to humans. Hence one could argue that soil health (also referred to as plant production, the soil fertility, soils habitat function, biodiversity pool) covers all the ecological soil functions[1]. These functions are capabilities of the soil to meet its full potential of supporting life and habitat in ecosystems by balancing water, carbon, nitrogen, oxygen and phosphorus cycling. By examining soil quality conditions for storing, filtering and transforming nutrients, substances and water, evaluation of soil health provides an evaluator with understanding about the threats to soil's capabilities of being a biodiversity pool for habitats, species and genes relevant for a particular ecosystem region. In the ecological

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[1] Soil health is usually defined as a capacity of the soil to function as a living system, to sustain biological productivity, promote environmental quality and maintain plant and animal health (Doran and Zeiss, 2000).

domain of sustainability and in line with the above reasoning, evaluation of the effects of remediation alternatives on soil functions is therefore related to soil health.

1.1.2   MCDA for sustainable remediation

The MCDA prototype was designed for sustainability appraisal of remediation alternatives (Rosén et al., 2009). There are several features that are important for practical application of the prototype, e.g:

  o   Structure for sustainability assessment

The structure captures fundamental criteria of the ecological and the socio-cultural domains of sustainability (Table 1.1), and a social profitability criterion in the economic domain (Rosén et al., 2008).

  o   Explicit accounting for different and sometimes conflicting criteria

The prototype addresses criteria and aspects often not evaluated in an open and transparent way. It accounts on views, goals and opinions of the various stakeholders (including representatives of the general public).

  o   Effective management of mixed data sets

Both qualitative and quantitative data, including expert knowledge judgments, can be effectively managed in the MCDA.

  o   Uncertainty analysis by Monte Carlo simulation

The prototype provides the opportunity to assess the confidence in the obtained results.

Table 1.1:   Key criteria for the ecological and the socio-cultural domains of sustainability (Rosén et al., 2009).

Ecological domain	Socio-cultural domain
Land environment	Equity and acceptance
Groundwater	Health due to contamination at the site
Surface water	Health due to remediation
Air	Cultural environment
Sediments	Recreation
Consumption of natural resources	Land use on site
	Land use off site

Initially, each remediation alternative is evaluated against sets of ecological and socio-cultural key criteria of the MCDA prototype. Each criterion is scored between -2 representing "very negative effect" and +2 representing "very positive effect" relative to a reference alternative. A score of 0 represents "no effect". Thereafter, the key criterion of the economic domain, social profitability, is investigated by means of a cost-benefit analysis (CBA) as specified by Rosén et al. (2008).

The MCDA prototype is based on a linear additive model (to rank the remediation alternatives) in combination with a non-compensatory method (to exclude those alternatives which are regarded as not leading towards sustainability). The most sustainable alternative is, according to the prototype, the one which generates the highest sustainability index in the interval [-1; +1]. The MCDA prototype is currently being further developed and parts of this work can be found in Norrman et al. (2012) and Rosén et al. (2013).

1.2   Scope and aim

The main objective of this report is to describe components and internal operations of the SF Box tool for soil function evaluation and to provide an illustrative example. The ultimate goal of the SF Box tool is to facilitate the input to sustainability appraisal of remediation alternatives by the MCDA model proposed by Rosèn et al. (2009). This input is a summary of the effects caused by remediation alternatives on ecological soil functions, where the effects are scored between -2 representing "very negative effect" and +2 representing "very positive effect". A score of 0 represents "no effect". The presented tool is relevant for evaluating the effects on the ecological functions of the upper soil layers (0-0.5m) within green areas of remediation sites.

1.3   Limitations

Soil function evaluation is based on a unified approach using soil quality indicators. However, the soil quality indicators are "function-dependent" (Lehmann and Stahr, 2010; Sojka and Upchurch, 1999). For example, the same soil quality indicator *soil texture* could be interpreted differently in linguistic variables: "good" for water filtering and "poor" for buffering of heavy metals, because the soil cannot perform these two functions good enough simultaneously. Although the confusion that may arise due to conflicting nature of some soil functions can be avoided by focusing on soil health evaluation (Idowu et al., 2008; Schindelbeck et al. 2008), there is still no standard "cross-functional" minimum data set (MDS) of the soil quality indicators for soil function evaluation. A great many of MDSs have been developed to meet agricultural land management needs (e.g. Andrews et al., 2004; Larson and Pierce, 1991; Reganold and Palmer, 1995; Singer and Ewing, 2000). Different MDSs have been suggested for soil evaluation for purposes other than agricultural productivity of the soil (Bone et al., 2010; Craul and Craul, 2006; Lehmann et al., 2008; Schindelbeck et al., 2008). The literature review was carried out to identify the most reasonable MDS for soil function evaluation in remediation projects (for details see Volchko et al., *in prep.*). The identified MDS consists of:

- soil texture;
- content of coarse material;
- organic matter content;
- available water capacity;
- pH;
- potentially miniralizable nitrogen;
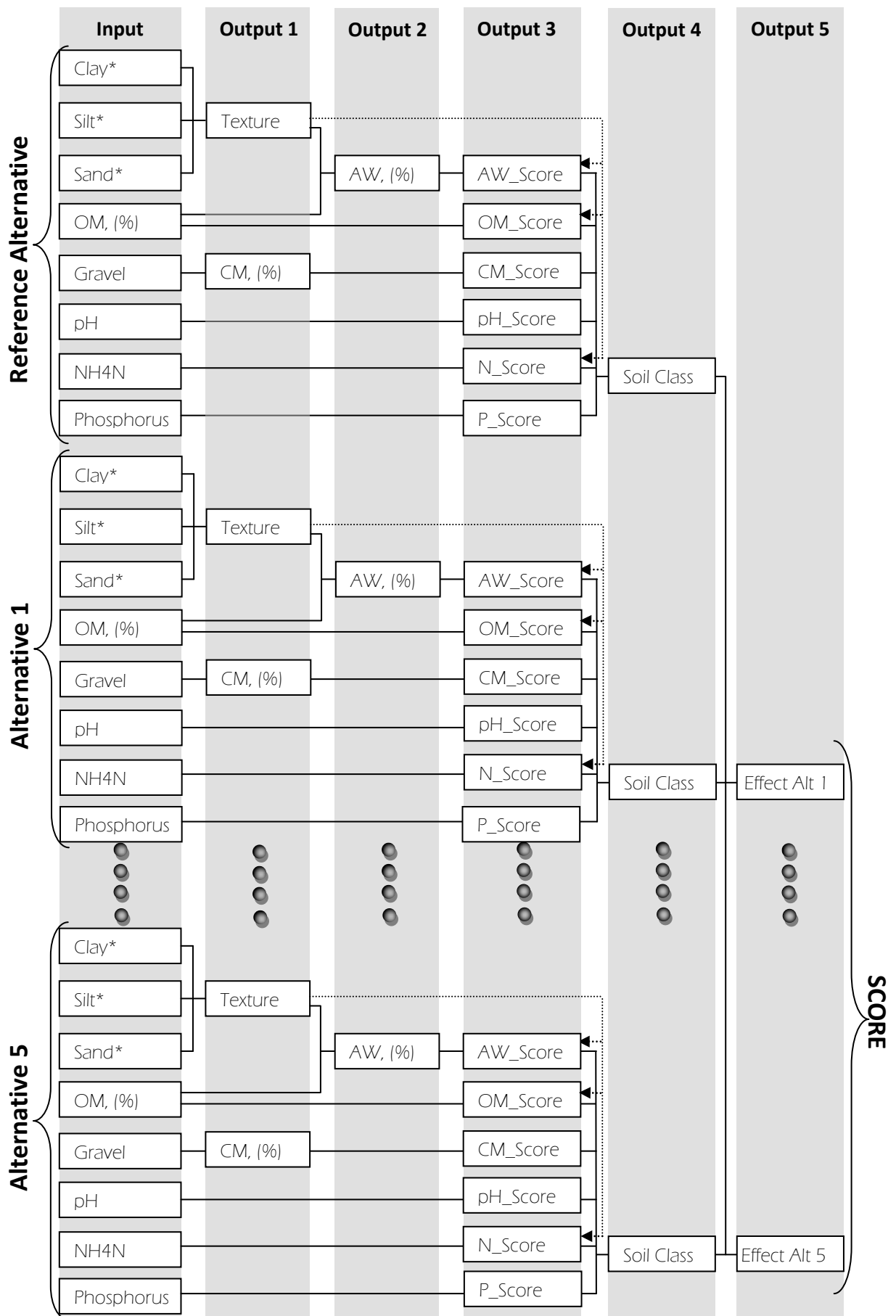- extractable phosphorus.

Figure 2.1:   The overall input/output flow in SF Box.

2 Description of the SF Box tool

SF Box is an Excel-based tool that contains seven sheets. These are SCORE, Reference Alternative, Alternative 1, Alternative 2, Alternative 3, Alternative 4, and Alternative 5. The SCORE sheet represents a summary of the effects caused by remediation alternatives on soil functions. These effects are calculated based on the changes in soil classes after remediation of contaminated land. The main output of the model in the Reference Alternative sheet is a soil class for the reference alternative (usually before remediation). The main output of the models in the Alternative 1, 2, 3, 4 and 5 sheets are the soil classes after alternative soil treatments. The overall algorithm for SF Box modeling is presented in Fig. 2.1. See also detailed description of the SF Box sheets in Sections 2.1-2.3.

2.1 SCORE

The outcome results of the SCORE sheet reflect the on-site effects after remediation for the Soil criterion in the ecological domain of the MCDA tool for sustainability appraisal of remediation alternatives (see the parts of the work in Norrman et al., 2011). In SF Box the SCORE sheet contains a summary of the effects caused by remediation alternatives (1, 2, 3, 4, and 5) on soil functions (see Fig. 3.5). The effects are scored between -2 representing "very negative effect" and +2 representing "very positive effect" relative to a reference alternative, e.g. when no action is taken (Rosén et al., 2009). A score of 0 represents "no effect". The effects of remediation alternatives on the soil functions are evaluated using a matrix of the effects relative to the reference soil class (Fig. 2.2). In this matrix, column "Reference Soil Class" represents the soil quality class which is calculated in the Reference Alternative sheet using input soil quality indicators and scoring functions (see description in Section 2.2). Row "Soil Class after Remediation" represents the soil quality class after remediation which is calculated in the Alternative 1 (2, 3, 4 and 5) sheet(s) of SF Box.
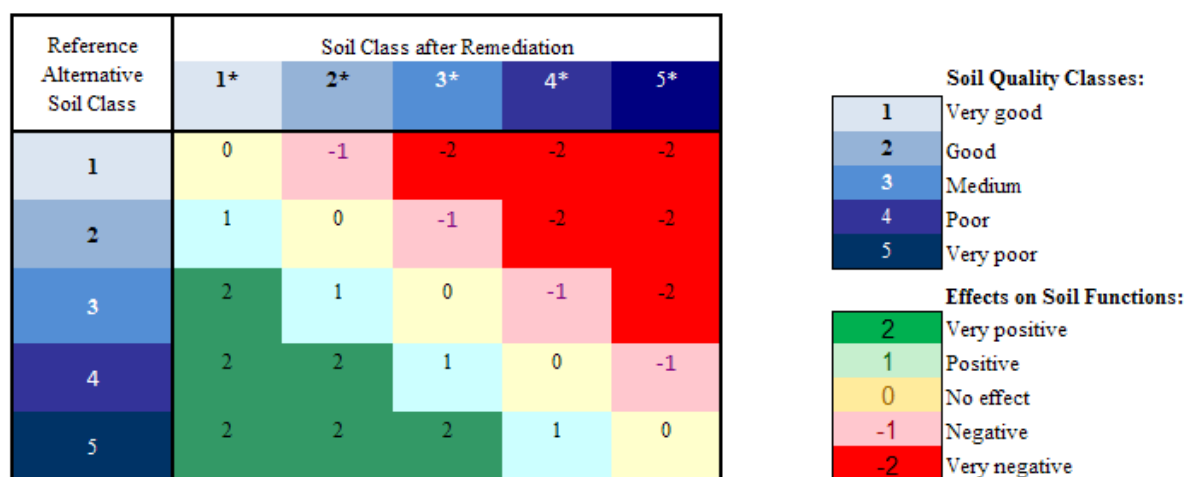

Figure 2.2:   Matrix of the Effects on Soil Functions.

Intensity of the effects on the soil functions are represented by different colors (green-light green-yellow-pink-red; see Fig. 2.2). The intensity of the soil function performance is represented on a blue scale as shown in Fig. 2.2, where darkest blue and lightest blue colors represent very poor and very good performances of soil functions respectively.

2.2 Reference Alternative

The Reference Alternative spreadsheet is modeled to compute the performance of soil functions using input soil quality indicators and scoring equations (see Section 2.2.3) which help to classify the soil into five classes ranging from "very poor" to "very good" quality (Cornell, 2009). An example of the SF Box spreadsheet model is presented in Fig. 3.1.

In SF Box, the cells for input parameters in a spreadsheet model are identified with bold font (Fig. 3.1). A brief description of inputs/outputs in the model is presented in Table 2.1.

Table 2.1:   Description of inputs and outputs in SF Box.

Inputs for SF Box	Description	Comment
Clay	Clay	The sum of input Clay [%], Silt [%], Sand [%], and Gravel [%] is equal to 100%. If the soil material contains ≤35% of gravel then the percentage contributions of clay, sand and silt to soil sample are recalculated using Equations 2.1-2.3. See detailed description in Section 2.2.1.
Silt	Silt	
Sand	Sand	
Gravel	Gravel	
OM [%]	Organic matter content	
pH	pH	
NH4-N [g/g per week] or [mg/kg]	Potentially mineralizable nitrogen	
P [mg/L][1] *or* [mg/kg]	Available phosphorus	

Inputs in dropdown menus	Description	Comment
Bulk Density [g/cm^3]	Bulk density of 1; 1.2; 1.4; 1.6; 1.8	The bulk density should be selected from a dropdown menu (the default value is 1.6 [g/cm^3] is set by) to enable SF Box computing available water capacity, AW [%].
Method for NH4-N	Anaerobic incubation St. methods	One of two available analysis methods (see references for the methods in Table 2.4) is selected from a dropdown menu to enable SF Box to compute N_Score.
Method for analysis phosphorus	Morgan-P Olsen-P AL-P Total P	One of the three available analysis methods (see references for the methods in Table 2.4) is selected from a dropdown menu to enable SF Box computing P_Score.

Inputs in dropdown menus	Description	Comment
Method for calculating the index	Arithmetic mean Quadratic mean Geometric mean	One of three available methods is selected from a dropdown menu to enable SF Box computing SF_Index.
Outputs for SF Box	**Description**	**Comment**
CM (%)	Content of coarse material	Content of coarse material is equal to gravel content, i.e. the amount of particles with $\phi > 2$mm.
Texture_Code	FAO and SGF texture codes	Texture_Code is determined using FAO soil taxonomy triangle if $CM \leq 35\%$ (Lehmenn et al., 2008; Appendix A) or SGF texture nomogram if CM>35% (SGF, 1984; Appendix C).
Texture_Name	FAO and SGF texture names	
AW (%)	Available water capacity	Available water capacity is a function of the texture code, organic matter content and bulk density. The bulk density is selected from a dropdown menu.
CM_Score	Score for coarse material content	The upper threshold content of coarse material for soil functioning is 35%. The lower threshold of a good quality is about 20% of coarse material (see details in Craul and Craul, 2006).
OM_Score	Score for organic matter content	
N_Score	Score for potentially mineralizable nitrogen	
P_Score	Score for available phosphorus	
Index	Soil function index for each sample	
Outputs for SF Box	**Description**	**Comment**
Performance	Soil function performance	SF_Performance and Soil Class are determined using Table 2.5.
Soil Class	Soil class	
N	Number of observations	Summary statistic for inputs and outputs.
m	Arithmetic mean	
s	Standard deviation	
P-95	95-percentile	
Max	Maximum	
VC	Coefficient of variation	

2.2.1 Output 1 (Soil Texture and Content of Coarse Material)
– Output: CM [%]/ Input: Gravel

Content of coarse material, CM (%), is automatically computed by SF Box and equals the content of gravel (i.e. particles ∅>2 mm). Content of coarse material is considered as an important soil quality indicator for soil functions, because if there are more than 35 % of particles larger than 2 mm, then the material is not classified as soil (Craul and Craul, 2005). Note, coarse-textured materials are gravel, sandy gravel, silty clayey gravel, sandy silty gravel, gravely sand, sand, loamy sand, sandy loam. Medium-textured materials are loam, silt loam, silt, sandy clay loam. Fine-textured materials are clayey loam, silty clayey loam, sandy clay, silty clay, clay (Cornell, 2009).

– Output: Texture_Code/ Input: Gravel, Sand, and the sum of Clay and Silt

Inputs for Gravel, Sand, Clay and Silt are automatically normalized to percentages, i.e. scale of input data (grams, kilograms or %) does not affect texture identification. The only requirement is to use the same scale for the gravel, sand, clay and silt contents in a soil sample. The sum of Gravel, Sand, Silt and Clay always generates 100%. If the content of coarse material CM [%] > 35% then Texture_Code is determined using SGF nomogram (SGF, 1984; Appendix B). Gravel, Sand, and the sum of Clay and Silt, i.e. fine material in SGF nomogram, is then used as input parameters for Texture_Code computation. If CM [%] ≤ 35% then Texture_Code is identified using the FAO Taxonomy Triangle, where the sides correspond to the contents of Clay*, Silt*, and Sand* in a soil sample (Lehmann et al., 2008; Appendix A). Clay*, Silt*, and Sand* recalculated automatically so that their sum equals to 100%:

$$Clay* \ [\%] = \frac{Clay[\%] \times 100\%}{Clay[\%] + Silt[\%] + Sand[\%]}, \tag{2.1}$$

$$Silt* \ [\%] = \frac{Silt[\%] \times 100\%}{Clay[\%] + Silt[\%] + Sand[\%]}, \tag{2.2}$$

$$Sand* \ [\%] = \frac{Sand[\%] \times 100\%}{Clay[\%] + Silt[\%] + Sand[\%]}. \tag{2.3}$$

A decision algorithm for the point-in-polygon problem is used in this study for computation of the soil texture code (see detailed description in Appendix A). The point-in-polygon problem asks whether a given point in the plane lies inside, outside, or on the boundary of a polygon. Point location problems widely applied in areas that deal with processing geometrical data, e.g. computer graphics (Preparata and Shamos, 1985).

2.2.2 Output 2 (Available Water Capacity)
– Output: AW [%]/ Input: Texture_Code, OM [%], and bulk density

Available water capacity is a function of texture code, organic matter content and bulk density. The available water capacity, AW [%], is computed using a table for the

determination of pore volume contents of mineral soils as specified by Lehmann et al. (2008) (see Appendix B).

2.2.3 Output 3 (Sub-scores, Soil Function Performance and Soil Class)

Sub-scores (i.e. CM_Score, OM_Score, AW_Score, pH_Score, N_Score, P_Score, and P_Score) are computed using scoring functions *f(x)* that transform input values of soil quality indicators into fractional numbers between 0 and 1, where 0 represents the poorest soil quality and 1 represents the best soil quality (Appendix D). For example, 12 mg P/L would be transformed by a scoring function into P_Score = 0.97 corresponding to "good soil quality" (see Appendix D, a graph for Morgan-P). Available water capacity of 5% would be transformed by another scoring function into AW_Score = 0.16 corresponding to "poor soil quality" (see Appendix D, a graph for available water capacity).

All the sub-scores are highlighted with help of green-yellow-red colors depending on the calculated values as specified in Table 2.3. Sub-scores in interval [0; 0.3] highlighted with red, in interval [0.31; 0.7] highlighted with yellow, and in interval [0.71; 1] highlighted with green correspond to "poor soil quality", "medium soil quality" and "good soil quality" respectively (Cornell, 2009).

Table 2.3:   Color palette for calculated sub-scores (Cornell, 2009).

Sub-score, (S)	Soil Quality
1≥ S >0.7	Good
0,7 ≥S >0.3	Medium
0,3≥ S ≥0	Poor

Transformation from input values to fractional numbers between 0 and 1 is done to enable a user to:

(1)   normalize input soil quality indicators, i.e. bringing the data from different scales (e.g. percentages and mg kg^{-1}) into one scale – fractional numbers in interval [0; 1];

(2)   interpret the input data in the context of soil functions, e.g. 2 mg Morgan-P L^{-1} corresponds to score of 0.46, i.e. "medium soil quality" for providing soil functions, whereas 33 mg Morgan-P L^{-1} corresponds to score of 0.19, i.e. "poor soil quality".

In this study, three types of scoring curves, i.e. "more is better", "optimum" and "less is better" are used for scoring as suggested by Andrews et al. (2004) and Cornell Soil Health Test (Cornell, 2009) (Fig. 2.3). For the "more is better" example, the higher the value of soil quality indicator the higher the performance score of this indicator. For "less is better" example, the lower the value of soil quality indicator the higher the performance score. For "optimum" example, there is a limited range of values corresponding to a high score, whereas "less" and "more" than this optimum values are scored lower.

Scoring functions are determined using an approximation method (similar to a test on goodness-of-fit of a statistical model) using the Grapher^{TM} software. The objective of the method is to make the approximation as close as possible to the actual function describing the relationship between the measured value of soil quality indicator and soil performance.
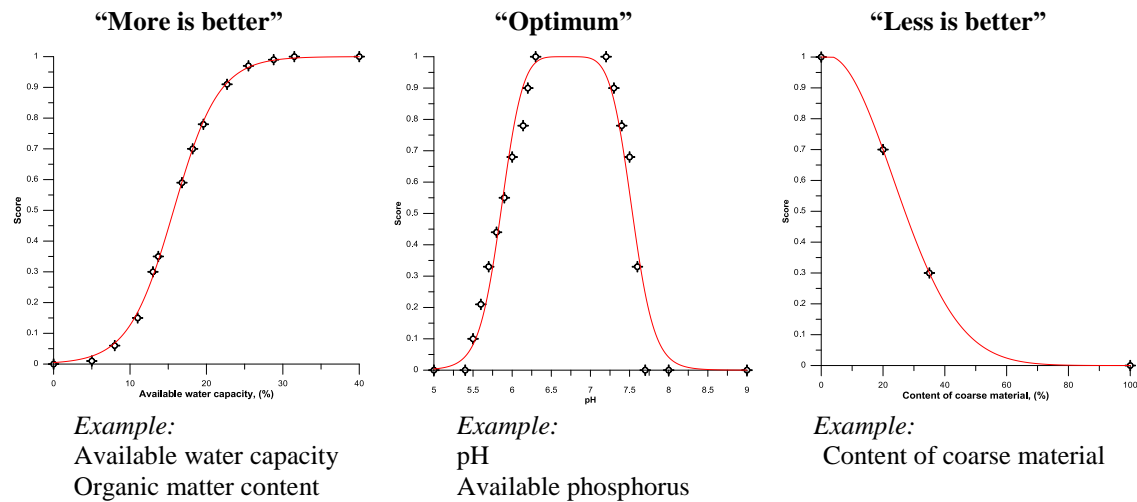
"More is better"	"Optimum"	"Less is better"

Example:
Available water capacity
Organic matter content

Example:
pH
Available phosphorus

Example:
Content of coarse material

Figure 2.3:   *Examples of scoring functions used for the interpretation of measured values of soil quality indicators (Andrews et al., 2004).*

The soil performance is described by (1) linguistic variables "good soil quality", "medium soil quality", "poor soil quality", and (2) scores, i.e. fractional numbers between 0 and 1, corresponding to these linguistic variables. In this study, the approximation is accomplished by using Gaussian, sigmoid, bell-shaped and linear functions (see Appendix D). The data on relationships (correlations) between the measured values of soil quality indicators and soil performances are provided in the literature sources (Table 2.4).

All the sub-scores are integrated into a soil function index that corresponds to the soil function performance and one of five soil classes (see Table 2.5). SF Box provides the possibility to determine a soil function index using three methods, i.e. computation of quadratic mean, arithmetic mean and geometric mean.

(1)   Quadratic mean:

$$Index = \sqrt{\frac{CM\_Score^2 + OM\_Score^2 + AW\_Score^2 + N\_Score^2 + P\_Score^2 + pH\_Score^2}{6}}$$

. (2.4)

(2)   Arithmetic mean:

$$Index = \frac{CM\_Score + OM\_Score + AW\_Score + N\_Score + P\_Score + pH\_Score}{6}.$$

(2.5)

(3) Geometric mean:

$$Index = \sqrt[6]{CM\_Score \times OM\_Score \times AW\_Score \times N\_Score \times P\_Score \times pH\_Score}.$$

(2.6)

Table 2.4:   Sources of data for determination of scoring functions.

Sub-Scores	Analysis Method	Scoring function type	Source of data for fit function determination
CM_Score	Sieving (ISO 3310-2:1999)	"Less is better"	The threshold value for soil functions (i.e. Score=0.3) is content of coarse material more than 35%. The lower limit of a good quality (i.e. Score=0.7) is about 20% of coarse material (see details in Craul and Craul, 2006).
OM_Score	Loss on ignition (SS-EN 12879)	"More is better"	The correlation between the measured content of organic matter and OM_Score is determined by Cornell (2009).
pH_Score	pH (H_2O) (ISO 10390)	"Optimum"	The correlation between the measured pH and pH_Score is determined by Cornell (2009).
AW_Score	Determination of pore volume contents of soils based on FAO soil texture, organic matter content and bulk density (Lehmann et al., 2008)	"More is better"	The correlation between the estimated available water and AW_Score is determined by Cornell (2009).
N_Score	Anaerobic incubation (Parfitt et al., 2005)	"More is better"	The correlation between the measured NH4-N and N_Score is determined by Cornell (2009).
	Standard Methods 18th Ed., 4500 NH_3-B		The scoring function follows the same shape as that for the anaerobic incubation method. The estimated representative values are provided by a certified laboratory that uses Standard Methods 18th Ed., 4500 NH_3-B for determination of potentially mineralizable nitrogen in the soil.
P_Score	Morgan-P (McIntosh, 1969)	"Optimum"	The correlation between the Morgan-P values and P_Score are determined by Cornell (2009).
	Olsen-P (ISO 11263)		The scoring function follow the same shape as that for Morgan-P. The agronomic optimum values of Olsen-P (15.2-26.4 mg/kg) and AL-P (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).
	AL-P (Egner et al., 1960)		
	Total P		

A color identification code for soil function performance is presented in Table 2.5 (see for example Fig. 3.1). Soil performances are classified into five classes as recommended by the Cornell Soil Health Test (Cornell, 2009).

Table2. 5:Correspondence between Soil Classes, Soil Function Performances and the total soil function index.

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

2.2.4 Output 4 (Summary Statistics)

Using standard functions available in MS Excel, some basic statistics is computed for input and output values (see Table 2.1 and Fig. 3.1).

2.3 Alternatives 1, 2, 3, 4 and 5

All the other sheets of the SF Box tool (i.e. A1, A2, A3, A4, and A5) are modeled to compute the performance of soil functions using the same input soil quality indicators and scoring functions as specified above in Section 2.2. Thus, all the spreadsheet models are programmed identically.

3 An example of SF Box application

This section provides an example of SF Box application for evaluation of the effects on soil functions in remediation projects. First the soil functions are evaluated for each alternative (including a reference alternative) in Section 3.1 (see detailed description of procedure in Section 2.2). Thereafter the effects on soil functions for each alternative are evaluated relative to the reference alternative in Section 3.2 (see description of procedure in Section 2.1). Section 3.3 presents an example of uncertainty analysis for the results obtained in Section 3.1 and Section 3.2.

Let us assume that there are three available remediation alternatives:

1. Excavation of the entire area, disposal of contaminated masses to a land fill, following by refilling with a clean material from sandpit 1.

2. Excavation of the entire area, disposal of contaminated masses to a land following by refilling with a clean material from sandpit 2.

3. Classifying the site as "Environmental Risk Area", i.e. delimiting the entire site with fences to prohibit visitors from entering the site, and thus assuming no soil remediation.

The reference alternative is "no action", i.e. leaving the area contaminated as it is at the present time.

3.1 Soil function evaluation for each remediation alternative

3.1.1 Reference alternative *(No action)*

In order to characterize the soil function performance for the reference alternative, 18 soil samples were collected at the site and analyzed with respect to the following soil quality indicators:

- Content of clay, silt, sand and gravel (using sieving and hydrometer methods);
- Organic matter content (using the loss on ignition method);
- Bulk density of 1.6 g cm^{-3} (using standard methods);
- pH (5:1 proportion of H_2O:soil);
- Potentially mineralizable nitrogen (Standard methods);
- Available phosphorus (Total P method).

All the data for 18 samples are inserted into appropriate input cells in the Ref sheet of SF Box (Fig. 3.1).

Appropriate methods are selected from drop down menus for available phosphorus (i.e. Total P), potentially mineralizable nitrogen (St. methods), and for soil function index computation (Arithmetic mean) (Fig. 3.2).

Label	Clay	Silt	Sand	Gravel	Code	Name	CM, (%)	CM_Score	OM, (%)	OM_Score	AW, (%) Bulk density 1.6	AW_Score	pH	pH_Score	NH4-N (mg/kg) Method St. methods	N_Score	P (mg/kg) Method Total P	P_Score	Index Method Arithmetic mean	Performance
1	0	2	81	17	S	Sand	17	0.78	0.8	0.07	21	0.87	8	0.04	180	0.01	460	0.81	0.43	Poor
2	0	2	89	9	S	Sand	9	0.95	0.7	0.07	21	0.87	7.1	0.99	180	0.01	460	0.81	0.62	Medium
3	0	1	93	6	S	Sand	6	0.99	1.6	0.16	22	0.90	6.5	1.00	180	0.01	420	1.00	0.68	Medium
4	0	0	79	20	S	Sand	20	0.70	7	0.99	24	0.93	8.2	0.01	230	0.06	440	1.00	0.61	Medium
5	0	2	79	19	S	Sand	19	0.73	3.2	0.52	22	0.90	6.3	0.99	220	0.04	520	0.33	0.59	Medium
6	0	2	88	10	S	Sand	10	0.93	3.7	0.66	22	0.90	6.4	1.00	170	0.01	480	0.53	0.67	Medium
7	11	14	73	2	SL	Sandy loam	2	1.00	5.8	0.95	25	0.95	6.5	1.00	210	0.03	700	0.01	0.66	Medium
8	0	3	82	15	S	Sand	15	0.83	0.6	0.06	21	0.87	6.7	1.00	170	0.01	390	0.76	0.59	Medium
9	0	1	84	15	S	Sand	15	0.83	1.5	0.15	22	0.90	6.1	0.89	170	0.01	380	0.52	0.55	Medium
10	0	2	80	18	S	Sand	18	0.76	0.8	0.07	21	0.87	6.4	1.00	170	0.01	420	1.00	0.62	Medium
11	11	16	70	3	SL	Sandy loam	3	1.00	6	0.96	25	0.95	5.6	0.14	210	0.03	730	0.01	0.51	Poor
12	0	2	77	21	S	Sand	21	0.67	5.4	0.92	24	0.93	6.5	1.00	210	0.03	430	1.00	0.76	Good
13	0	2	82	16	S	Sand	16	0.81	1.5	0.15	22	0.90	6.3	0.99	180	0.01	390	0.76	0.60	Medium
14	0	3	80	17	S	Sand	17	0.78	3.4	0.58	22	0.90	6.2	0.95	140	0.00	460	0.81	0.67	Medium
15	0	5	78	16	S	Sand	16	0.80	0.9	0.08	21	0.87	5.8	0.41	180	0.01	520	0.33	0.42	Poor
16	3	10	83	4	LS	Loamy sand	4	1.00	4.4	0.80	25	0.95	5.9	0.60	230	0.06	580	0.08	0.58	Medium
17	0	1	80	19	S	Sand	19	0.73	1.2	0.11	22	0.90	6	0.77	160	0.01	370	0.29	0.47	Poor
18	0	5	91	4	S	Sand	4	1.00	1	0.09	21	0.87	7.5	0.60	170	0.01	460	0.81	0.56	Medium

		Number of observations (N)	18	18	18	18	18	18	18	18	18	18	18		
N		Number of observations (N)	18	18	18	18	18	18	18	18	18	18			
m		Mean (m)	0.85	2.75	0.41	22.39	0.90	6.56	0.74	186.67	0.02	478.33	0.60	0.59	Medium
s		Standard deviation (s)	0.12	2.16	0.38	1.50	0.03	0.72	0.36	25.44	0.02	101.53	0.35		
P-95		95-persentile (P-95)	1.00	6.15	0.96	25.00	0.95	8.03	1.00	230.00	0.06	704.50	1.00		
Max		Maximum (Max)	1.0	7.0	1.0	25.0	0.9	8.2	1.0	230.0	0.1	730.0	1.0		
VC		Coefficient of variation (VC)	0.14	0.78	0.92	0.07	0.03	0.11	0.48	0.14	0.80	0.21	0.58		

Soil Class 3

Ref / A1 / A2 / A3 / A4 / A5 / SCORE / BD distribution

Figure 3.1:   Computation results for Reference alternative.

A bulk density of 1.6 g/cm^3 is set by default in SF Box (Fig. 3.1). However, four other options are available in a dropdown menu (Fig. 3.2 (a)). The sub-scores for content of coarse material, organic matter content, available water, pH, potentially mineralizable nitrogen and available phosphorus are computed automatically for each soil sample and colored with red-yellow-green depending on the generated sub-scores.
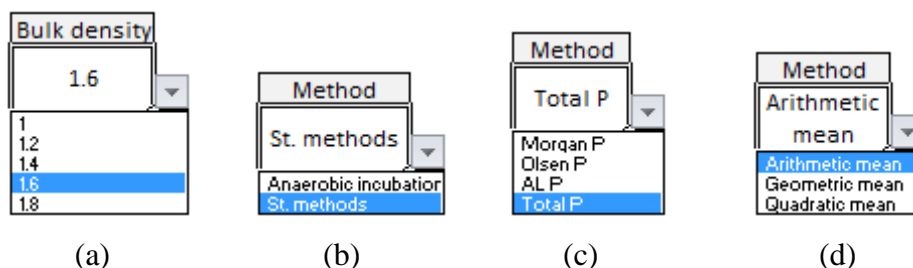

| (a) | (b) | (c) | (d) |

Figure 3.2:   Dropdown menus in SF Box for (a) available water capacity, (b) potentially mineralizable nitrogen, (c) available phosphorus, and (d) soil function index.

All the sub-scores are thereafter integrated into soil function indices and soil function performances for each soil sample (see AE and AF columns of the spreadsheet model in Fig. 3.1). Finally, a resulting soil class of 3 (medium soil performance) is computed for the entire site based on the mean index, which is equal to 0.59 (cell AC27 of the spreadsheet model in Fig. 3.1). Summary statistics for each soil quality indicator and each sub-score is also computed automatically (see rows 26-31 of the spreadsheet model in Fig. 3.1).

3.1.2   **Alternative 1** *(Refilling with a soil from sandpit 1)* **& Alternative 2** *(Refilling with a soil from sandpit 2)*

Alternatives 1 and 2 assume that after excavation and disposal of contaminated masses to a land fill, the entire site will be refilled with a clean material. For Alternative 1 a resulting class of 1 (very good soil function performance) is computed for the entire site based on the mean index, which is equal to 0.93 (cell AC27 of the spreadsheet model in Fig.3.3). For Alternative 2 a resulting class of 4 (poor soil function performance) is computed for the entire site based on the mean index, which is equal to 0.49 (cell AC27 of the spreadsheet model in Fig.3.4)

3.1.3   **Alternative 3** *(Classifying as "Environmental Risk Area")*

This remediation alternative coincides with the Reference Alternative *(No action)*.

Label	Clay	Silt	Sand	Gravel	Code	Name	CM, (%)	CM_Score	OM, (%)	OM_Score	AW, (%)	AW_Score	pH	pH_Score	NH4-N (mg/kg)	N_Score	P (mg/kg)	P_Score	Index	Performance
											Bulk density 1.6				Method St. methods		Method Total P		Method Arithmetic mean	
1	0	2	81	17	S	Sand	17	0.78	7	0.99	24	0.93	6.8	1.00	400	0.91	460	1.00	0.94	Very good
2	0	2	80	18	S	Sand	18	0.76	7.2	0.99	24	0.93	6.8	1.00	400	0.91	460	1.00	0.93	Very good
N				Number of observations (N)			2	2	2	2	2	2	2	2	2	2	2	2		
m				Mean (m)			0.77	7.10	0.99	24.00	0.93	6.80	1.00	400.00	0.91	460.00	1.00		0.93	Very good
s				Standard deviation (s)			0.02	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
P-95				95-persentile (P-95)			0.78	7.19	0.99	24.00	0.93	6.80	1.00	400.00	0.91	460.00	1.00			
Max				Maximum (Max)			0.8	7.2	1.0	24.0	0.9	6.8	1.0	400.0	0.9	460.0	1.0			
VC				Coefficient of variation (VC)			0.02	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00			

Soil Class 1

Figure 3.3:   Computation results for Alternative 1 (Excavation & Refilling with a clean material from sandpit 1).

Label	Clay	Silt	Sand	Gravel	Code	Name	CM, (%)	CM_Score	OM, (%)	OM_Score	AW, (%)	AW_Score	pH	pH_Score	NH4-N (mg/kg)	N_Score	P (mg/kg)	P_Score	Index	Performance
											Bulk density 1.6				Method St. methods		Method Total P		Method Arithmetic mean	
1	0	0	44	56	saGr	Sandy gravel	56	0.04	0	0.03	21	0.87	6.8	1.00	0	0.00	430	1.00	0.49	Poor
2	0	0	40	60	saGr	Sandy gravel	60	0.02	0	0.03	21	0.87	6.8	1.00	0	0.00	420	1.00	0.49	Poor
N				Number of observations (N)			2	2	2	2	2	2	2	2	2	2	2	2		
m				Mean (m)			0.03	0.00	0.03	21.00	0.87	6.80	1.00	0.00	0.00	425.00	1.00		0.49	Poor
s				Standard deviation (s)			0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	7.07	0.00			
P-95				95-persentile (P-95)			0.04	0.00	0.03	21.00	0.87	6.80	1.00	0.00	0.00	429.50	1.00			
Max				Maximum (Max)			0.0	0.0	0.0	21.0	0.9	6.8	1.0	0.0	0.0	430.0	1.0			
VC				Coefficient of variation (VC)			0.34	0.00	0.00	0.00	0.00	0.00		0.00	0.00	0.02	0.00			

Soil Class 4

Figure 3.4:   Computation results for Alternative 2 (Excavation & Refilling with a clean material from sandpit 2).

3.2 Evaluation of the effects on soil functions

The effect of remediation alternatives on soil functions are summarized in the SCORE sheet (Fig. 3.5).

Figure 3.5: *Computation results reflecting the effects of remediation alternatives on soil functions (Copy of a sheet from the SCORE© tool).*

Note that soil function indices for all the alternatives in the above example are computed using the arithmetic mean method (see Section 2.2.3) as suggested by Andrews et al. (2004). SF Box allows for sensitivity analysis of the computed indices by choosing one of three computational methods from a dropdown menu (see Fig. 3.2 (d)). The result of a sensitivity analysis for the above example is presented in Table 3.1.

Table 3.1: Sensitivity analysis of the obtained results: Effects of remediation alternatives on soil functions using different methods for soil index computation.

| No | Alternative | Method for computation of the soil function index | | | | | | | | |
| | | Arithmetic | | | Quadratic | | | Geometric | | |
		I	C	E	I	C	E	I	C	E
0	Reference	0.59	3	---	0.71	2	---	0.30	5	---
1	Refilling with a soil from sandpit 1	0.93	1	**+2**	0.94	1	**+2**	0.93	1	**+2**
2	Refilling with a soil from sandpit 2	0.49	4	**-1**	0.68	3	**0**	0.06	5	**-2**

I: Soil function index.
C: Soil class.
E: Effects of remediation alternative on soil functions.

Depending on the selected computation method for the soil function index, Alternative 1 *Refilling with a soil from sandpit 1* generates a score of +2 reflecting a very positive effect on soil functions.

Alternative 2 *Refilling with a soil from sandpit 2* generates scores -1, 0, -2 when soil function index is computed by arithmetic, quadratic and geometric mean methods respectively.

Logically, Alternative 3 *Classifying as "Environmental Risk Area"* always generates a score of 0, corresponding to no effects on soil function.

3.3 Uncertainty analysis

Being an Excel-based tool, SF Box allows for uncertainty analysis using Monte Carlo Simulation by the Oracle Crystal Ball[©] add-in software. This section provides an example of uncertainty analysis for the results obtained in Section 3.1. Simulation is performed on the spreadsheet models of SF Box for SCORE effects, Reference Alternative, Alternative 1 *Refilling with a soil from sandpit 1* and Alternative 2 *Refilling with a soil from sandpit 2*. Uncertainty analysis for Alternative 3 *Classifying as "Environmental Risk Area"* was omitted because this alternative assumes no remedial action and, as a consequence, results in no changes in soil class relative to the reference alternative.

In order to run a simulation, the statistical assumptions of input variables and the forecasts output results have been defined in the simulation model. Assumptions are the uncertain independent variables in the spreadsheet models of SF Box. These are contents of clay, silt, sand, and gravel; organic matter content; bulk density; pH; potentially mineralizable nitrogen; and available phosphorus. Forecast cells contain formulas and combine the values in the assumptions to calculate a result (CB, 2007). The forecast cells in SF Box are soil classes in the spreadsheet models, and computed effects in the SCORE sheet. A probability distribution is selected from a distribution gallery in Oracle Crystal Ball[©] and assigned to each assumption (uncertain variable). In this example, lognormal and custom distributions are assigned to variables (see shapes of these distributions in Fig. 3.6).
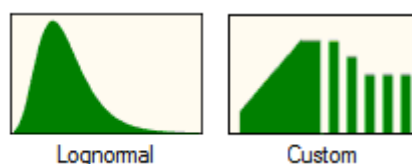

Figure 3.6:   Distribution types used in this study (CB, 2007).

A lognormal distribution is selected for variables with known but uncertain values, because the values of all soil quality indicators are always positive.

Table 3.2:   Assigned distributions to variables in the spreadsheet models of the SF Box tool.

Assumptions	Remediation Alternatives		
	Reference	Refilling with a soil from sandpit 1	Refilling with a soil from sandpit 2
Clay, Sand, Silt, Gravel	L	L	L
Organic matter content	L	L	L
Bulk Density	C	C	C
pH	L	L	L
Potentially mineralizable nitrogen	L	L	L
Available phosphorus	L	L	L

L: Lognormal distribution.
C: Customized distribution.

The most likely bulk density is 1.6 g/cm^3, the distribution has a shape as presented in Fig. 3.7.
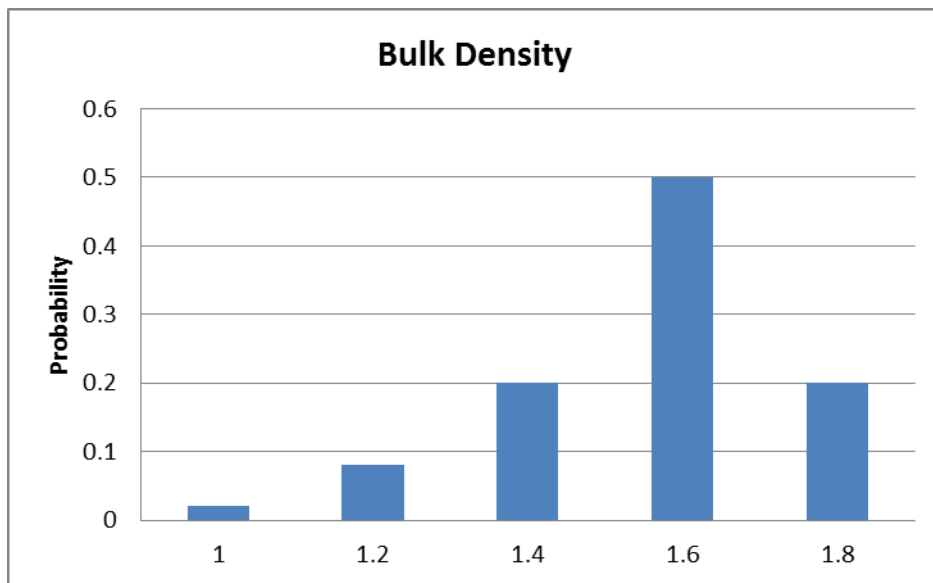

Figure 3.7: *Probability distribution of soil bulk density for Reference Alternative.*

When assumptions and forecasts have been defined, Monte Carlo simulation (with 10 000 trials) is applied using the Oracle Crystal Ball$^©$ add-in software.

The results of Monte Carlo simulation for computed soil function indices are presented in Fig. 3.8, showing the 5th percentile, the mean and the 95th percentile of the simulated soil function index.

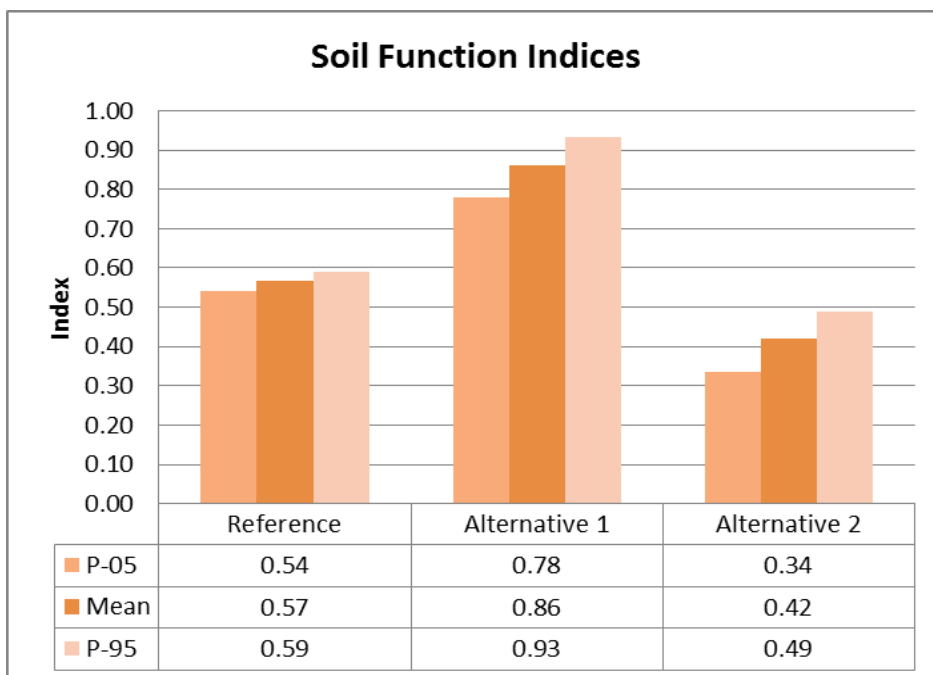|	Reference	Alternative 1	Alternative 2
P-05	0.54	0.78	0.34
Mean	0.57	0.86	0.42
P-95	0.59	0.93	0.49

Figure 3.8: Results of the uncertainty analysis for the computed soil function indices.

The uncertainty analysis for the effects of remediation alternatives on soil functions (i.e. scores in the SCORE sheet of SF Box) is combined with sensitivity analysis of

the obtained results (Fig. 3.9). Using the Oracle Crystal Ball[©] add-in software, the sensitivity analysis was done to see contribution from each input variable of the spreadsheet model to the total uncertainty in the resulting scores (Fig. 3.10).
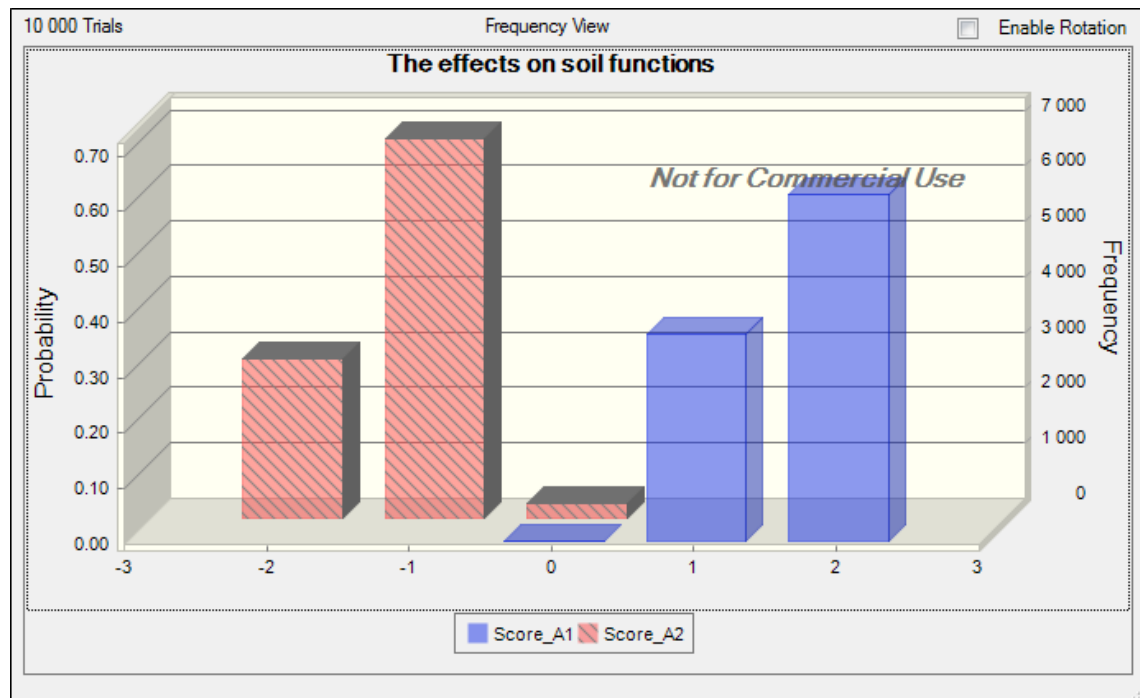

Figure 3.9: Results of the uncertainty analysis for the resulting scores (i.e. the effects on soil functions). Score_A1 – the resulting scores for Remediation Alternative 1. Score_A2 – the resulting scores for Remediation Alternatives 2.
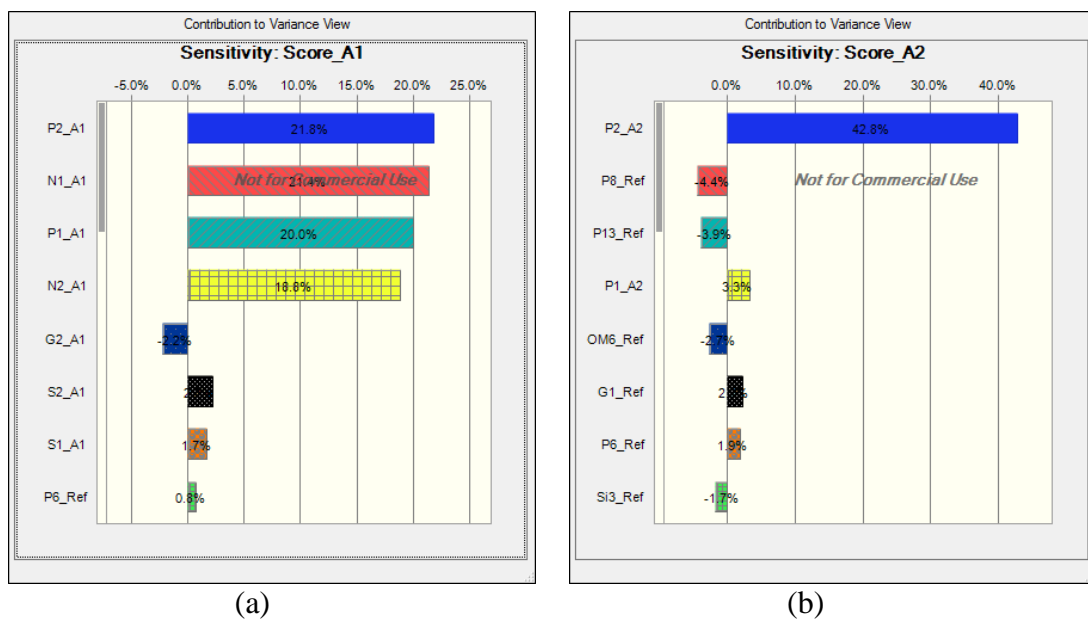

Figure 3.10: The contribution of variables to the total uncertainty in the resulting scores. Score_A1 – the resulting scores for Remediation Alternative 1. Score_A2 – the resulting scores for Remediation Alternatives 2.

4   Discussion

This report describes the components and internal operations of the SF Box tool for evaluating effects on soil functions, including an example. The developed SF Box tool could assist in soil function evaluation in remediation projects to meet emerging regulatory requirements on soil protection, the proposed EU Soil Framework Directive (COM, 2006). The results of the SF Box tool are complementary to the environmental risk assessment in remediation projects. The focus of this discussion is on the computation of the resulting scores for the example described in Section 3. These scores between -2 and +2 represent the effects of remediation alternatives on ecological functions of the upper soil layers.

The procedure for soil function evaluation includes a sequence of five steps:

(1) evaluation of sub-scores for soil quality indicators;

(2) integration of these sub-scores into a soil function index;

(3) computation of a soil class for the entire site based on the mean soil function index;

(4) scoring the effects on soil functions (i.e. scoring a change in soil classes) relative to the reference alternative;

(5) uncertainty and sensitivity analyses of the resulting scores.

In this study soil classification is based on the arithmetic mean of sub-scores as suggested by Andrews et al. (2004), Cornell (2009), Idowu et al. (2008) and Schindelbeck et al. (2008). It is obvious that the resulting soil class is sensitive to the method used for integration of sub-scores for soil quality indicators (see Table 3.1). By providing options for computation of the arithmetic, the quadratic and the geometric means, the SF Box tool allows for the sensitivity analysis. This type of analysis was done in Section 3.2 to see the difference between the different ways of computing soil function indices.

Using the Oracle Crystal Ball$^©$ add-in software, another type of sensitivity analysis was done to identify the contribution from each input variable of the spreadsheet model to the total uncertainty in the resulting scores (Section 3.3, Fig. 3.10). Further, only positive scores are possible for Alternative 1 *Refilling with a soil from sandpit 1* and only negative scores are possible for Alternative 2 *Refilling with a soil from sandpit 2* (Fig. 3.9). *Available phosphorus* is the most sensitive variables in the spreadsheet model of the SF Box tool for the above mentioned alternatives (Fig. 3.10).

By assigning scores and handling the uncertainties in the scores, the SF Box tool could facilitate the input for sustainability appraisal with respect to the effects on ecological function of the upper soil layers within green areas of the remediation site. Since the effects of remediation alternatives on soil functions are associated with big uncertainties, it is more reasonable to assign probability distributions for the scores instead of discrete values within the MCDA model for sustainability appraisal of remediation alternatives, as this was suggested by Rosén et al. (2009), Norrman et al. (2012) and Rosén et al. (2013).

5   Concluding remarks

Being in line with the proposed EU Soil Framework Directive (COM, 2006), the SF Box tool is developed to facilitate the input with respect to the effects of remediation alternatives on ecological functions of the upper soil layers within green areas of remediation sites. This early version of the tool has its pros and cons. On the one hand *available water capacity* is computed automatically, which is an advantage. On the other hand, if this soil quality indicator was determined using a standard laboratory methods, it would not be possible to insert available data manually. Another constraint of the tool is associated with bulk density options in a dropdown menu. The model only uses discrete bulk density values in interval [1; 1.8].

To the advantage of a user the tool provides:

- Color visualization of outputs.

Identification of soil function performances as well as sub-scores with different colors helps a user to readily interpret the results saving time and efforts.

- Flexibility.

The dropdown menus are developed to provide a user with some flexibility on selection among standard methods (*i*) used for laboratory analysis of the soil quality indicators, and (*ii*) to be applied for computation of soil function index.

- Monte Carlo simulation opportunities.

Being en Excel-based tool, the SF Box tool allows for uncertainly analysis of the obtained results using Monte Carlo simulation provided by the Oracle Crystal Ball© software.

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Appendices

Appendix A   Algorithm for FAO soil texture computation

FAO soil texture is an expression of the relative amounts of sand, silt, and clay in a soil. The soil texture is displayed in a triangular graph known as the FAO soil textural triangle (Fig. A1).
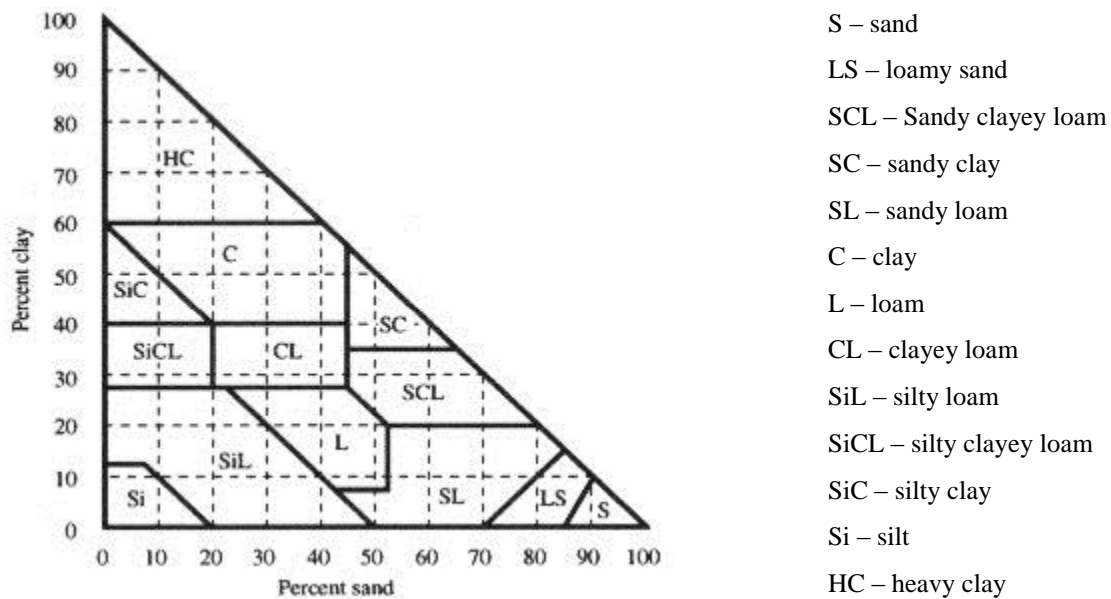

S – sand

LS – loamy sand

SCL – Sandy clayey loam

SC – sandy clay

SL – sandy loam

C – clay

L – loam

CL – clayey loam

SiL – silty loam

SiCL – silty clayey loam

SiC – silty clay

Si – silt

HC – heavy clay

Figure A.1:   FAO soil taxonomy triangle.

In this triangle, two axes arranged at 90 degree angle represent the composition of the soil in terms of its percentage of sand and clay. The hypotenuse of this triangle represents the percentage of silt. A soil that is purely clay would correspond to percentages of Clay-Silt-Sand (100-0-0) while pure sand would correspond to percentages of Clay-Silt-Sand (0-0-100). The total of all constituents cannot exceed 100%. Loam that is near the center of the triangle might then correspond to percentages of Sand-Silt-Clay around (33-33-33).

Algorithm for texture computation is based on a solution for the point-in-polygon problem (PIP) (Preparata and Shamos, 1985).

1. Consider two axes representing the contents of sand and clay in a FAO soil taxonomy triangle are X- and Y-axes of a coordinate system (Figure A.2).

2. As the soil texture codes are delimited by lines forming simple polygons, the regular polygons have been formed by determining coordinates of their vertices going *clockwise*. For example, the vertices for polygon number 1 {A, B, C} are A (0; 100), B (40; 60), and C (0; 60) (Figure A.2). The non-simple polygons of texture codes SiL and SL have been however divided in order to form simple ones (red lines in Figure A.2). As a result, 15 regular simple polygons are formed to enable solving PIP.

3. To ease the computation procedure, the polygons have been grouped into three blocks depending on the number of vertices (Fig. A.2; block 1: polygons 1, 2, 3, 4; block 2: polygons 5, 6, 7, 8, 9, 10, 11; and block 3: polygons 12, 13, 14).
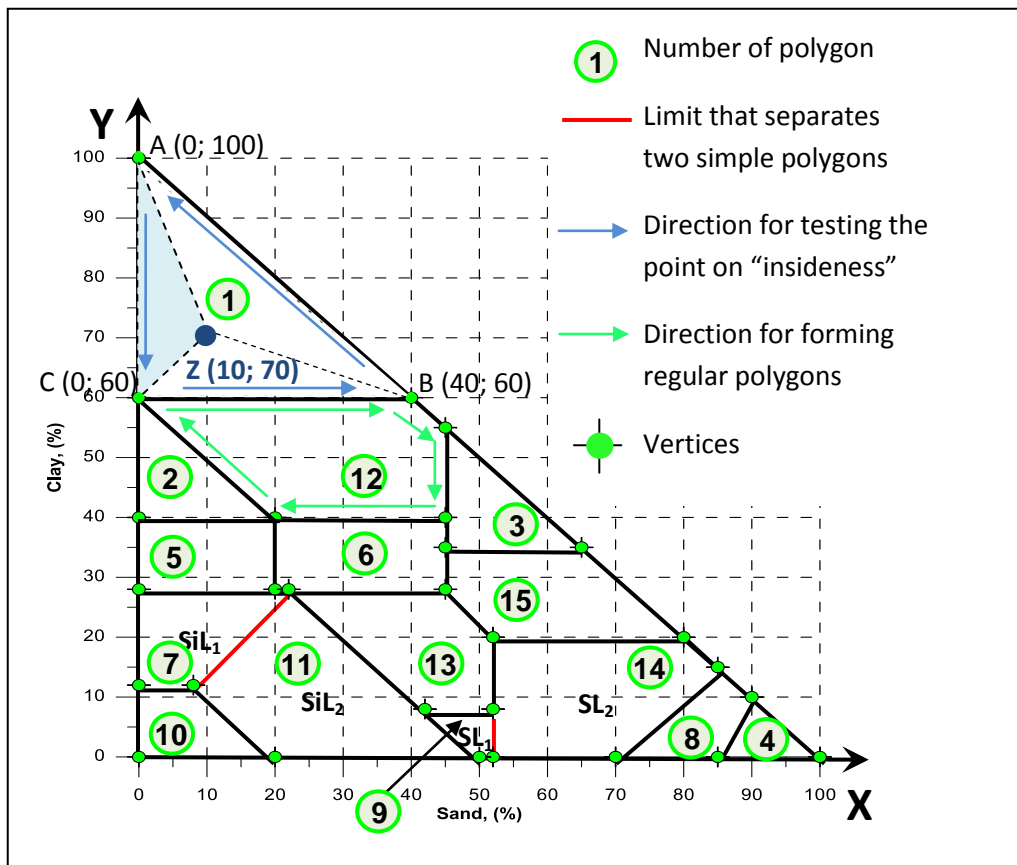
Figure A.2:   A graph of plotted polygons for FAO soil texture codes.

4. The algorithm determines if a given point (x, y) is inside of a given polygon by: (*a*) drawing a pair of rays from that point to the vertices $(x_1; y_1)$ and $(x_2; y_2)$; and (*b*) checking if determinant, det (*A*), for this pair is positive:

$$\det \ (A) = \begin{vmatrix} x & y & 1 \\ x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \end{vmatrix} = x(y_1 - y_2) - y(x_1 - x_2) + (x_1 y_2 - x_2 y_1)$$

(Preparata and Shamos, 1985).

Starting from and finishing by the first vertex of a given polygon, the determinants are tested on "positiveness" until all vertices of this polygon are visited in a *counterclockwise* manner. If at list one of the determinants is negative, the point is outside of the tested polygon. If all determinants are positive, the point is inside of the polygon. If determinant is zero, the point lies on the edge of polygon. If other determinants for this polygon are positive then the point is considered as being inside.

Example: Does a soil sample comprising of 10% sand and 70% clay belong to soil texture class "Heavy clay"?

1. Heavy clay expression in a FAO taxonomy triangle corresponds to polygon 1 in Figure A.2. The vertices of polygon are points A (0; 100), B (40; 60), and C (0; 60). Let us test if point Z (10; 70) corresponding to a soil sample composition (sand; clay) is inside of this polygon.

2. Let us draw rays from point Z (x; y) and visit all the vertices of the polygon pairwise in a counterclockwise manner (starting from and ending by point A, i.e. the first vertex of the polygon) (Figure A.2).

3. Let us calculate determinants for pairs:

(*i*) ZA and ZC,

$$\begin{vmatrix} 10 & 70 & 1 \\ 0 & 100 & 1 \\ 0 & 60 & 1 \end{vmatrix} = 10(100-60)-70(0-60)+(0 \cdot 60 - 0 \cdot 100) = 400.$$

(*ii*) ZC and ZB,

$$\begin{vmatrix} 10 & 70 & 1 \\ 0 & 60 & 1 \\ 40 & 60 & 1 \end{vmatrix} = 10(60-0)-70(40-60)+(0 \cdot 60 - 40 \cdot 100) = 400.$$

(*iii*) ZB and ZA,

$$\begin{vmatrix} 10 & 70 & 1 \\ 40 & 60 & 1 \\ 0 & 100 & 1 \end{vmatrix} = 10(60-100)-70(40-0)+(40 \cdot 100 - 60 \cdot 0) = 800.$$

Answer: Since all determinants are positive, point Z (10; 70) is inside of the tested polygon. Sequently, the soil sample comprising of 10% sand and 70% clay belongs to soil texture class "Heavy clay".

Appendix B   Determination of available water capacity of mineral soils

Table A.1:   Determination of available water capacity of mineral soils (modified from Lehmann et al., 2008).

FAO TEXTURAL CLASS	Available water content, AW (%)				
	With bulk density [g cm⁻³]				
	1.0	**1.2**	**1.4**	**1.6**	**1.8**
Sand (S) 0%OM	**7**	**11**	**17**	**21**	**21**
Addition if 1-2% OM	8	12	18	22	22
if 2-4% OM	8	12	18	22	22
if 4-8% OM	10	14	20	24	24
if 8-15% OM	11	15	21	25	25
Loamy sand (LS) 0%OM	**12**	**17**	**20**	**22**	**21**
Addition if 1-2% OM	13	18	21	23	22
if 2-4% OM	13	18	21	23	22
if 4-8% OM	15	20	23	25	24
if 8-15% OM	16	21	24	26	25
Sandy loam (SL) 0%OM	**19**	**21**	**23**	**22**	**20**
Addition if 1-2% OM	20	22	24	23	21
if 2-4% OM	20	22	24	23	21
if 4-8% OM	22	24	27	25	23
if 8-15% OM	23	25	28	26	24
Sandy clayey loam (SCL)	**20**	**20**	**19**	**17**	**13**
Addition if 1-2% OM	21	21	20	18	14
if 2-4% OM	22	22	21	19	15
if 4-8% OM	25	25	24	21	18
if 8-15% OM	29	29	28	26	22
Clayey loam (CL)	**22**	**20**	**17**	**14**	**10**
Addition if 1-2% OM	23	21	18	15	11
if 2-4% OM	24	22	19	16	12
if 4-8% OM	27	25	22	19	15
if 8-15% OM	31	29	26	23	19
Silty clayey loam (SiCL)	**24**	**22**	**18**	**15**	**10**
Addition if 1-2% OM	25	23	19	16	11

if 2-4% OM	26	24	20	17	12
if 4-8% OM	29	27	23	20	15
if 8-15% OM	38	36	32	29	24
Sandy clay (SC) 0%OM	**34**	**33**	**31**	**27**	**22**
Addition if 1-2% OM	35	34	32	28	23
if 2-4% OM	35	34	32	28	23
if 4-8% OM	38	37	35	31	26
if 8-15% OM	39	38	36	32	27
Silty loam(SiL) 0%OM	**28**	**28**	**26**	**23**	**18**
Addition if 1-2% OM	29	29	27	24	19
if 2-4% OM	29	29	27	24	19
if 4-8% OM	32	32	30	27	22
if 8-15% OM	33	33	31	28	23
Loam(L) 0%OM	**24**	**24**	**23**	**20**	**16**
Addition if 1-2% OM	25	25	24	21	17
if 2-4% OM	26	26	25	22	18
if 4-8% OM	28	28	27	24	20
if 8-15% OM	31	31	30	27	23
Silt (S), Silty Clay(SiC)	**20**	**17**	**13**	**17**	**13**
Addition if 1-2% OM	22	19	15	19	15
if 2-4% OM	25	22	18	22	18
if 4-8% OM	31	28	24	28	24
if 8-15% OM	36	33	29	33	29
Clay(C) 0%OM	**14**	**11**	**8**	**14**	**10**
Addition if 1-2% OM	16	13	10	16	12
if 2-4% OM	19	16	13	19	15
if 4-8% OM	25	22	19	25	21
if 8-15% OM	30	27	24	30	26

Appendix C   SGF texture nomogram
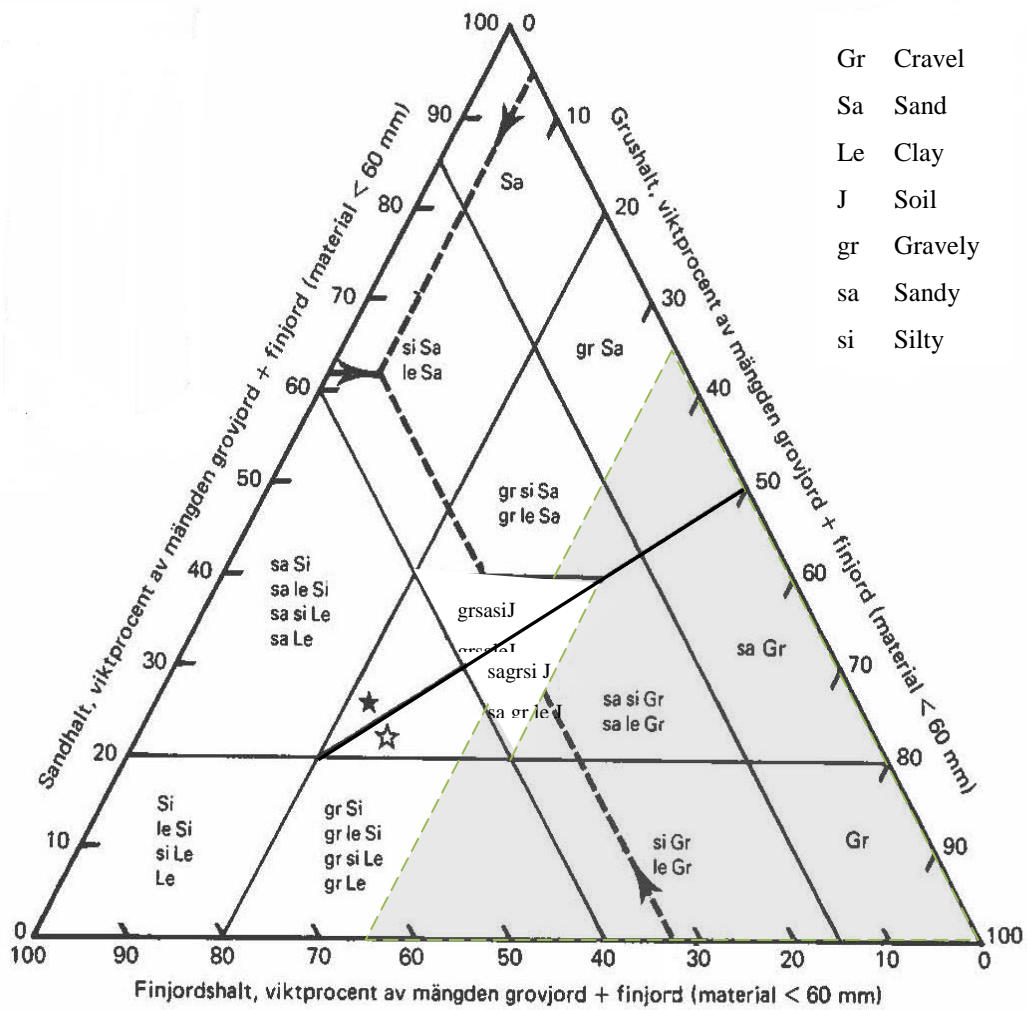
Figure C.1: Nomogram for classification of mineral soil without moraine (SGF, 1984): area colored with grey is used for soil texture determination if the content of coarse material >35% and the content of fine material (silt and clay) <65%.

Appendix D   Scoring equations for soil quality indicators

1. Organic matter content

Scores for organic matter content is calculated using sigmoid functions.
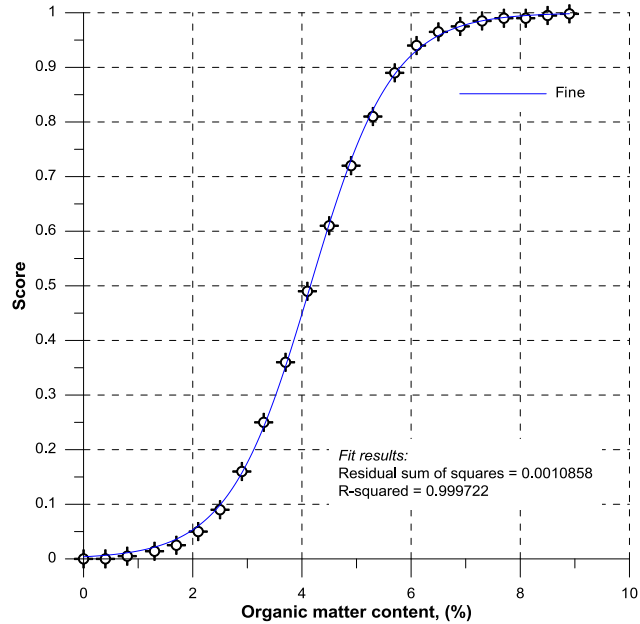
Scoring function for organic matter content in a fine-textured material:

$$f(x) = \frac{1}{1 + e^{-1.34(x-4.16)}} \; .$$
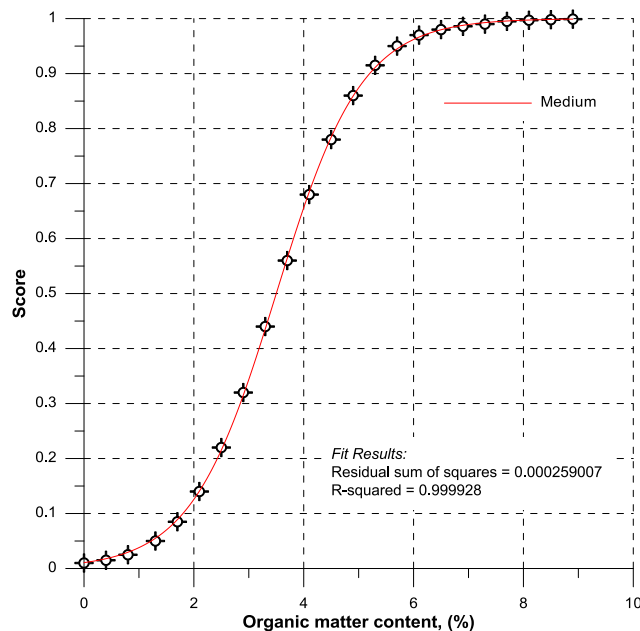
Scoring function for organic matter content in a medium-textured material:

$$f(x) = \frac{1}{1 + e^{-1.29(x-3.5)}} \; .$$
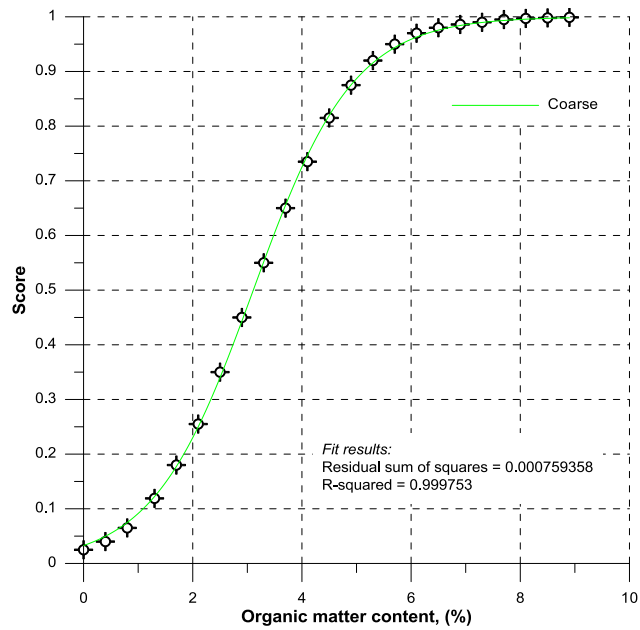
Scoring function for organic matter content in a coarse-textured material:

$$f(x) = \frac{1}{1 + e^{-1.09(x-3.11)}} \; .$$

2. Available water capacity

Scores for available water capacity is calculated using sigmoid functions.
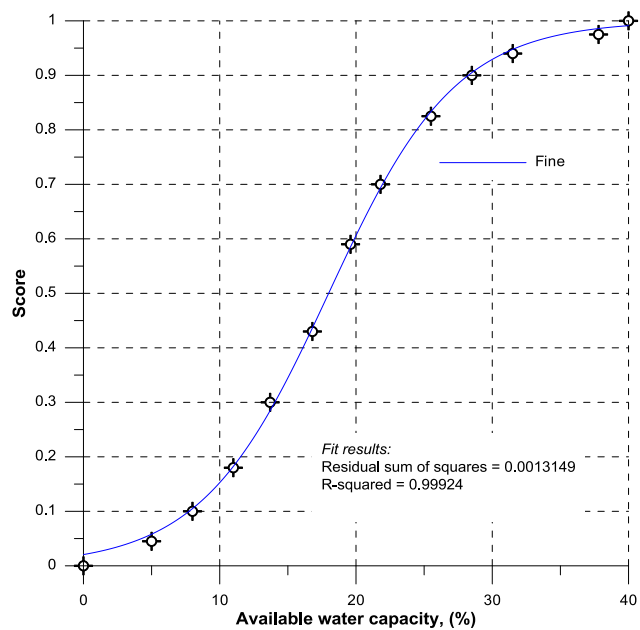
Scoring function for available water capacity in a fine-textured material:

$$f(x) = \frac{1}{1 + e^{-0.21(x-18)}} \; .$$
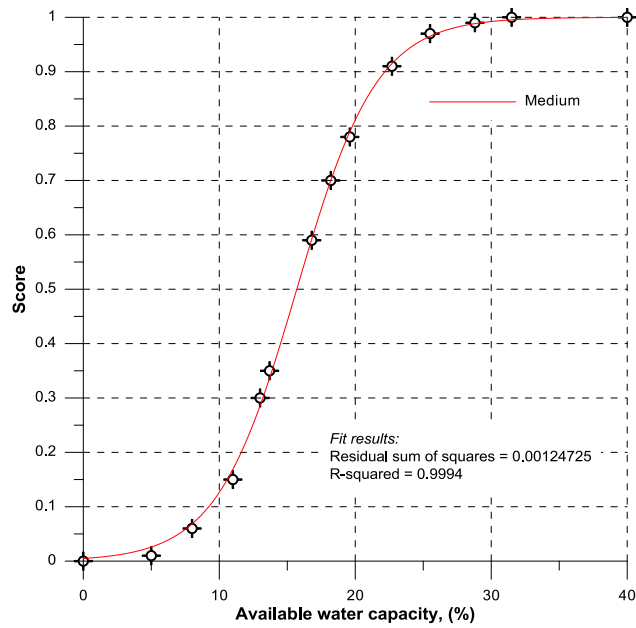
Scoring function for available water capacity in a medium-textured material:

$$f(x) = \frac{1}{1 + e^{-0.34(x-15.7)}} \ .$$
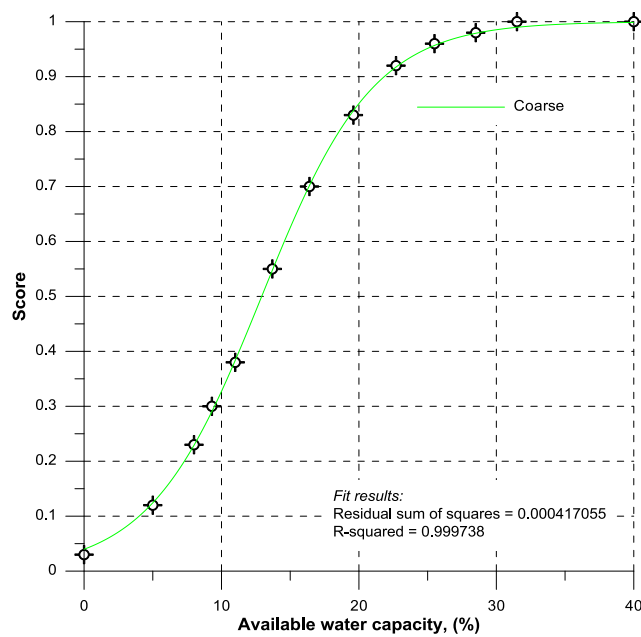
Scoring function for available water capacity in a coarse-textured material:

$$f(x) = \frac{1}{1 + e^{-0.24(x-12.9)}} \ .$$

3. Potentially mineralizable nitrogen
3.1.   Analysis method: *Anaerobic incubation*
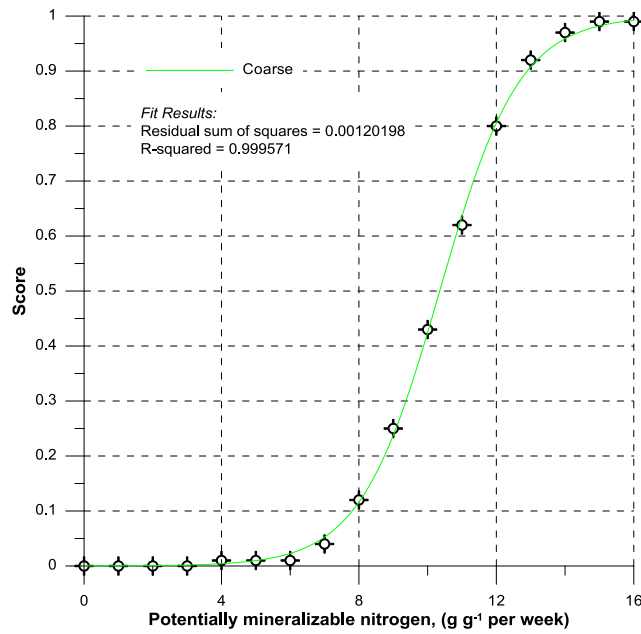
Scoring function for potentially mineralizable nitrogen in a coarse-textured material:

$$f(x) = \frac{1}{1 + e^{-0.86(x-10.35)}}\ .$$
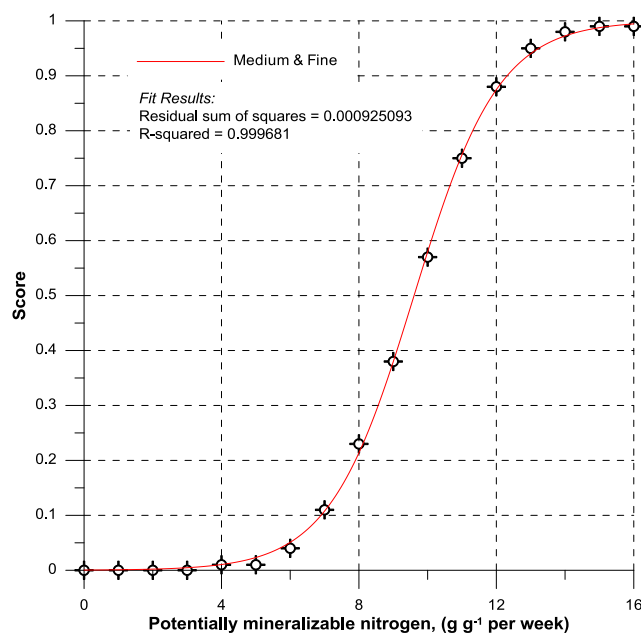
Scoring function for potentially mineralizable nitrogen in medium- and fine-textured materials:

$$f(x) = \frac{1}{1 + e^{-0.81(x-9.6)}}\ .$$

3.2.   Analysis method: *Standard methods 18th edition*
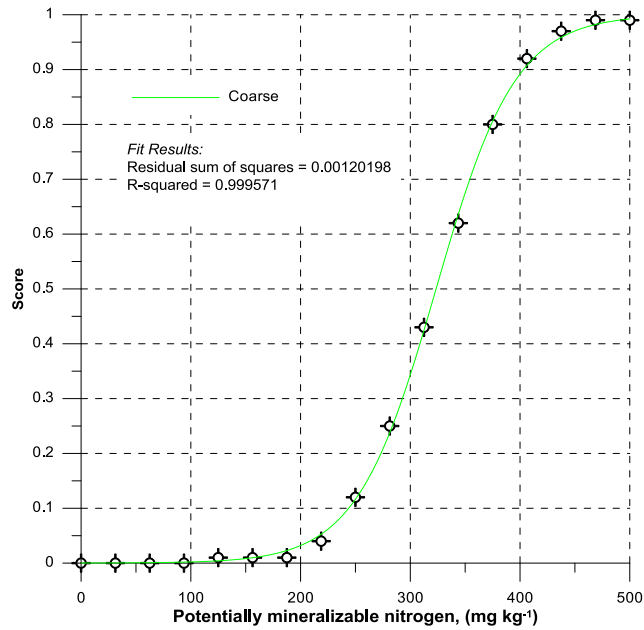
Scoring function for potentially mineralizable nitrogen in coarse-textured material:

$$f(x) = \frac{1}{1 + e^{-0.03(x - 323.49)}} \; .$$
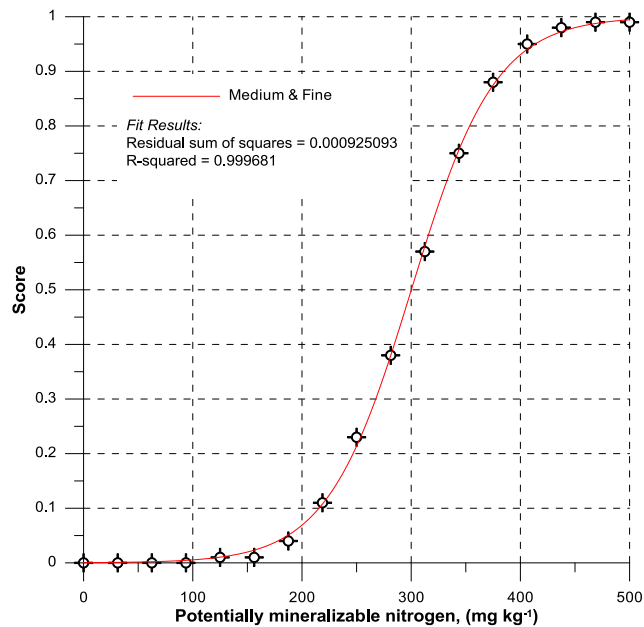
Scoring function for potentially mineralizable nitrogen in medium- and fine-textured materials:

$$f(x) = \frac{1}{1 + e^{-0.026(x - 300.14)}} \; .$$

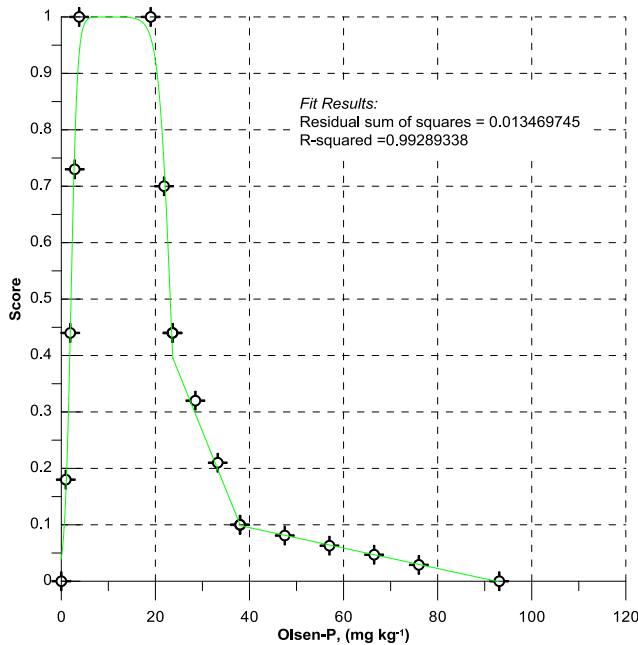## 4. Phosphorus
4.1. Analysis method: *Morgan-P*
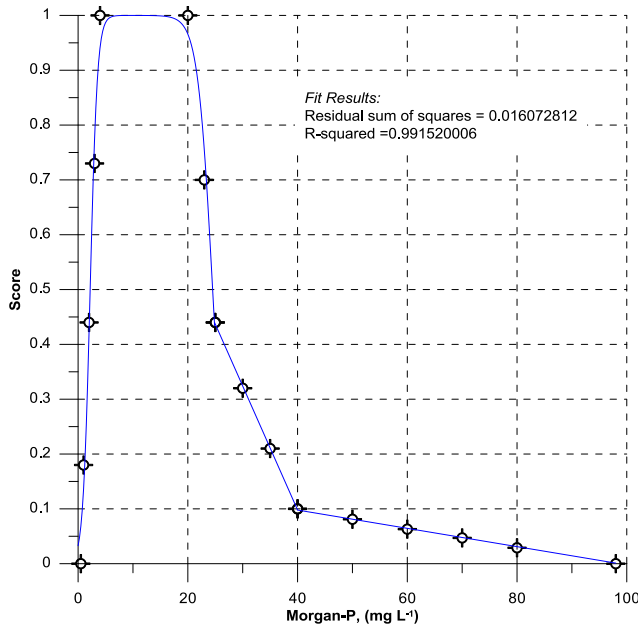
Optimum value:
4-20 mg Morgan-P L^{-1}.

Not-to-exceed value:
40 mg Morgan-P L^{-1}.

Scoring function for Morgan-P is a system of equations:

$$f(x) = \begin{cases} \dfrac{1}{1+e^{-1.54(x-2.198)}} - \dfrac{1}{1+e^{-0.74(x-24.52)}}, & 0 \le x \le 24.88; \\ -0.0226x + 1.002, & 24.88 < x \le 40; \\ -0.00167x + 0.165, & 40 < x \le 98; \\ 0, & x > 98. \end{cases}$$
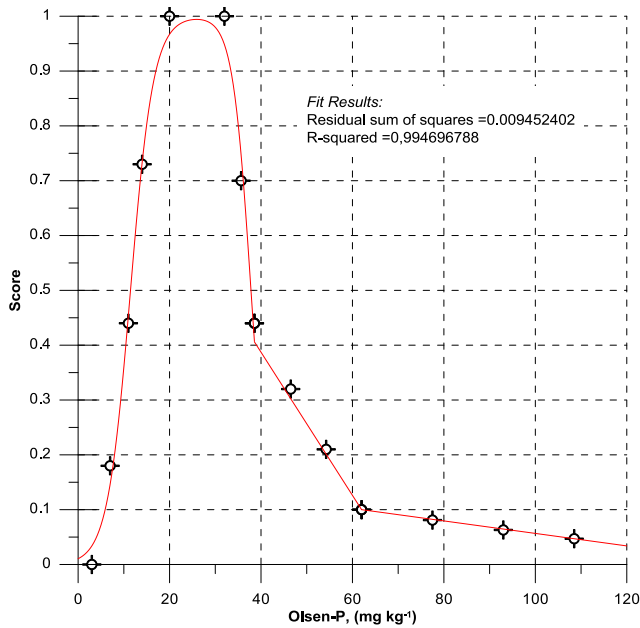
4.2. Analysis method: *Olsen-P*

Optimum value:
3-19 mg Olsen-P kg^{-1}.

Not-to-exceed value:
38 mg Olsen-P kg^{-1}.

Scoring function for Olsen-P in a coarse-textured soil:

$$f(x) = \begin{cases} \dfrac{1}{1+e^{-1.54(x-2.067)}} - \dfrac{1}{1+e^{-0.787(x-23.159)}}, & 0 \le x \le 23.7; \\ -0.02069x + 0.886, & 23.7 < x \le 338; \\ -0.0018x + 0.167, & 38 < x \le 92; \\ 0, & x > 92. \end{cases}$$
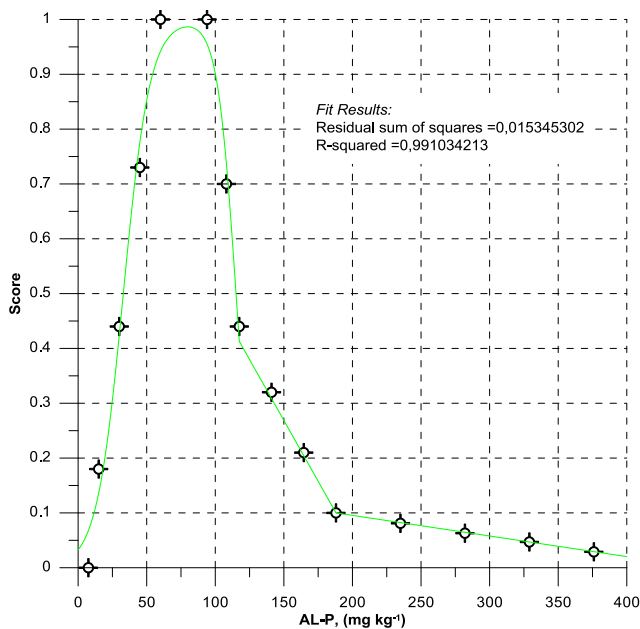
Optimum value:
20-32 mg Olsen-P kg^{-1}.

Not-to-exceed value:
62 mg Olsen-P kg^{-1}.

Scoring function for Olsen-P in a fine- and medium-textured soil:

$$f(x) = \begin{cases} \dfrac{1}{1+e^{-0.3963(x-11.457)}} - \dfrac{1}{1+e^{-0.502(x-37.809)}}, & 0 \le x \le 38.56; \\ -0.01306x + 0.91, & 38.56 < x \le 62; \\ -0.0011x + 0.17, & 62 < x \le 120; \\ 0, & x > 120. \end{cases}$$
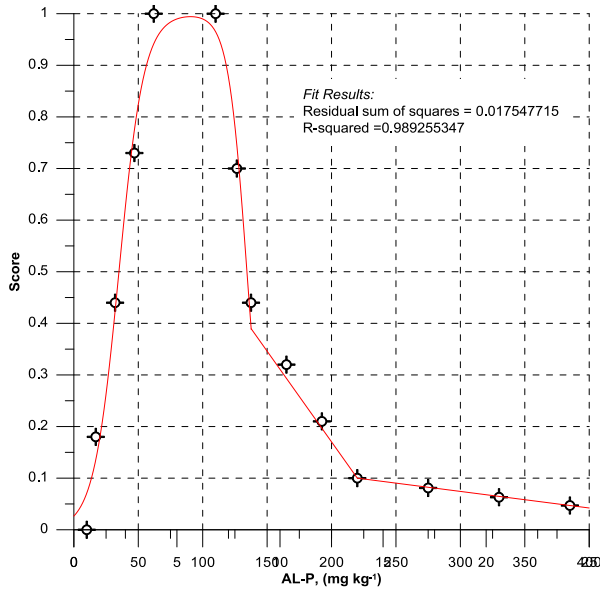
4.3. Analysis method: *AL-P*

Optimum value:
60-94 mg AL-P kg^{-1}.

Not-to-exceed value:
188 mg AL-P kg^{-1}.

Scoring function for AL-P in a coarse-textured soil:

$$f(x) = \begin{cases} \dfrac{1}{1+e^{-0.147(x-115.13)}} - \dfrac{1}{1+e^{-0.103(x-32.95)}}, & 0 \le x \le 117.55; \\ -0.00044x + 0.93, & 117.55 < x \le 188; \\ -0.00038x + 0.17, & 188 < x \le 360; \\ 0, & x > 360. \end{cases}$$
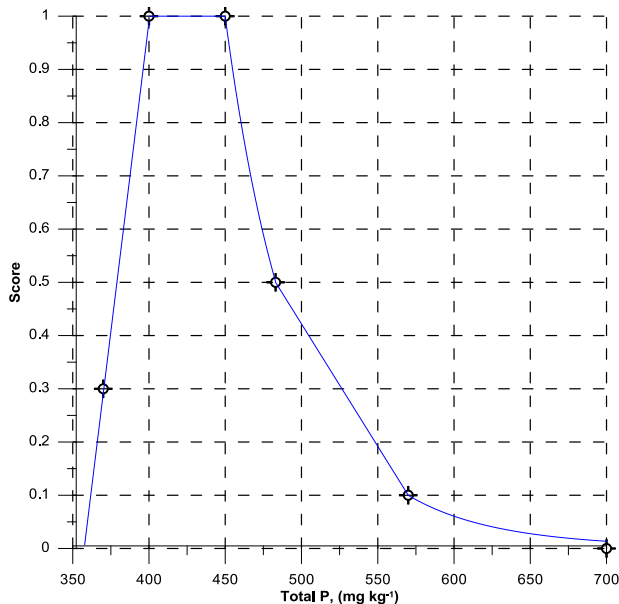
Optimum value:
62-100 mg AL-P kg^{-1}.

Not-to-exceed value:
220 mg AL-P kg^{-1}.

Scoring function for AL-P in medium- and fine-textured soils:

$$f(x) = \begin{cases} \dfrac{1}{1+e^{-0.137(x-13434)}} - \dfrac{1}{1+e^{-0.103(x-34.995)}}, & 0 \le x \le 137.66; \\ -0.0035x + 0.87, & 137.66 < x \le 220; \\ -0.00032x + 0.17, & 220 < x \le 360; \\ 0, & x > 360. \end{cases}$$
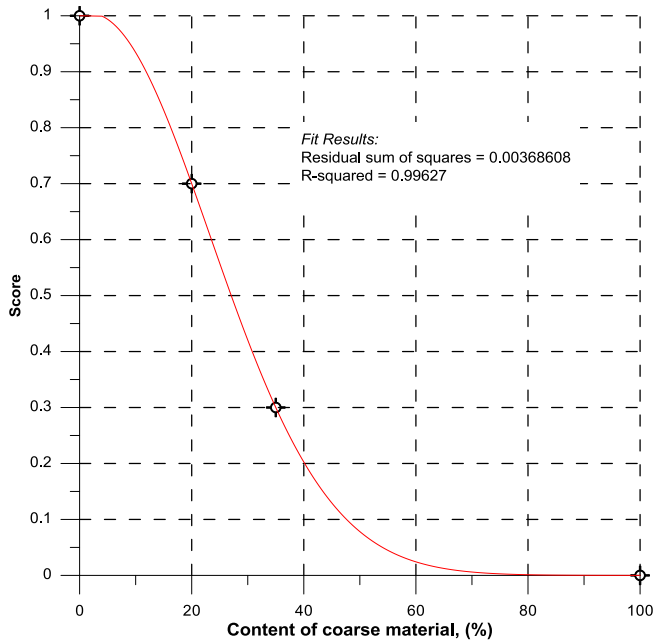
4.4. Analysis method: *Total P*

Low:	373 mg P kg^{-1}.
Medium:	483 mg P kg^{-1}.
Optimum:	411 mg P kg^{-1}.
Excessive:	571 mg P kg^{-1}.

Scoring function for Total P in soils:

$$f(x) = \begin{cases} 0.0233 \cdot x - 8.33, & 357 \le x < 400; \\ 1, & 400 \le x \le 450; \\ 6.8 \cdot 10^{25} \cdot x^{-9.7}, & 450 < x \le 483; \\ -0.0046 \cdot x + 2.72, & 483 < x \le 570; \\ 6.8 \cdot 10^{25} \cdot x^{-9.7} & x > 570; \\ 0, & x < 357. \end{cases}$$

5. Content of coarse material

Fit Results:
Residual sum of squares = 0.00368608
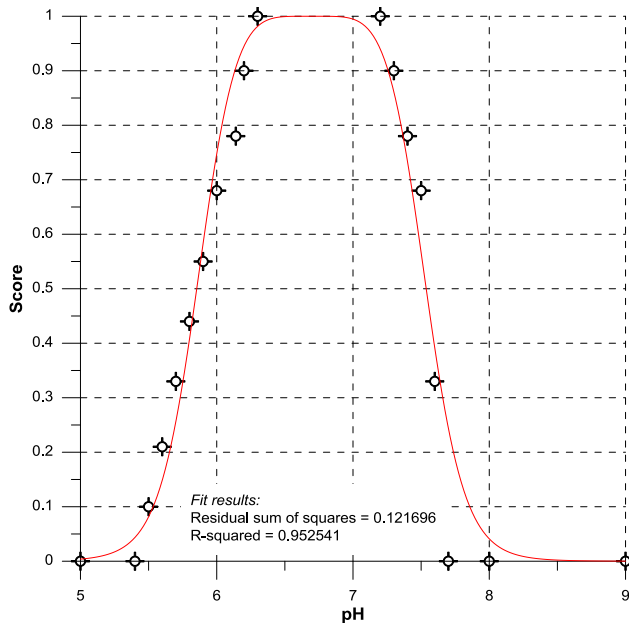R-squared = 0.99627

Comment: A score of 0.3 corresponds to 35% of coarse material; a score of 0.7 corresponds to 20% of coarse material (see details in Craul and Craul, 2005).

Scores are calculated using a modified Gaussian function:

$$f(x) = e^{\left(-\frac{11.04x^2}{10000} + \frac{0.43x}{100}\right)}.$$

6. pH

Fit results:
Residual sum of squares = 0.121696
R-squared = 0.952541

A score for pH is calculated using a bell-shaped function:

$$f(x) = \frac{1}{1 + |x - 6.7|^6} \cdot \frac{1}{1 + |x - 6.7|^5}.$$