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Soil quality — Characterization of contaminated soil related to groundwater protection

Qualité du sol — Caractérisation des sols pollués en relation avec la protection des eaux souterraines

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ISO copyright office
CP 401 • Ch. de Blandonnet 8
CH-1214 Vernier, Geneva
Phone: +41 22 749 01 11
Fax: +41 22 749 09 47
Email: copyright@iso.org
Website: www.iso.org

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Foreword

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The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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This document was prepared by Technical Committee ISO/TC 190, *Soil quality*, Subcommittee SC 7, *Impact assessment*.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

This second edition cancels and replaces the first edition (ISO 15175:2004), which has been technically revised.

The main change concerns the focus on contaminated land management. This second edition suggests a tiered approach from simple to complex assessment in order to evaluate the impact of soil contamination of groundwater.

Soil quality — Characterization of contaminated soil related to groundwater protection

1 Scope

This document provides guidance on the principles behind, and main methods for, the evaluation of sites, soils and soil materials in relation to their role as a source of contamination of groundwater and their function in retaining, releasing and transforming contaminants. It is focused on contaminated land management identifying and listing relevant monitoring strategies, methods for sampling, soil processes and analytical methods.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at http://www.electropedia.org/

3.1
aquifer
geological water-bearing formation (bed or stratum) of permeable rock, or unconsolidated material (e.g. sand and gravels) capable of yielding significant quantities of water

[SOURCE: ISO 5667-11:2009, 3.5]

3.2
contaminant
substance or agent present in the *soil* (3.10) as a result of human activity

Note 1 to entry: See *pollutant* (3.7).

Note 2 to entry: There is no assumption in this definition that harm results from the presence of the contaminant.

[SOURCE: ISO 11074:2015, 3.4.6, modified — a new Note 1 to entry has been added and the subsequent note has been renumbered.]

3.3
dissolved organic carbon
DOC
concentration of organic carbon remaining in solution after filtration and/or centrifugation under defined conditions

Note 1 to entry: Dissolved organic carbon is expressed in mg/l, g/m^3.

3.4
groundwater
water in the saturated zone of an underground geological formation or artificial deposit such as made ground, e.g. fill material

[SOURCE: ISO 5667-11:2009, 3.9, modified — “and/or unsaturated zone” has been removed.]

3.5
water table
upper boundary surface of the *groundwater* (3.4)

[SOURCE: ISO 11074:2015, 3.2.4]

3.6
percolating water
infiltrating water that moves downward in the pore space due to gravity

[SOURCE: ISO 11074:2015, 3.2.5]

3.7
pollutant
substance or agent present in the *soil* (3.10) [or *groundwater* (3.4)] which, due to its properties, amount or concentration causes adverse impacts on *soil functions* (3.11) or soil use

[SOURCE: ISO 11074:2015, 3.4.18, modified — “or soil use” has been added.]

3.8
pore water
water in the pores or cavities within a body of rock or *soil* (3.10)

[SOURCE: ISO 5667-11:2009, 3.18, modified — “water that fills the pores” has been replaced by “water in the pores”.]

3.9
risk assessment
process of risk analysis and evaluation of the damaging effects on humans and the environment, with respect to the nature, extent, and probability of occurrence of these effects

[SOURCE: ISO 11074:2015, 5.2.26, modified — “effects on man” has been replaced by “effects on humans”.]

3.10
soil
upper layer of the Earth's crust composed of mineral particles, organic matter, water, air and organisms

Note 1 to entry: In a broader civil engineering sense, soil includes topsoil and sub-soil; deposits such as clays, silts, sands, gravels, cobbles, boulders, and organic matter and deposits such as peat, materials of human origin such as wastes, ground gas and moisture, and living organisms.

[SOURCE: ISO 11074:2015, 2.1.11, modified — “transformed by weathering and physical/chemical and biological processes” has been removed.]

3.11
soil function
description of the significance of *soils* (3.10) to man and the environment

EXAMPLE Control of substance and energy cycles as compartment of ecosystems, basis for the life of plants, animals, and man, basis for the stability of buildings and roads, basis for the yield of agriculture, horticulture, and forestry, carrier of genetic reservoir, document of natural history, archaeological and paleoecological document.

[SOURCE: ISO 11074:2015, 3.3.31]

3.12
soil gas
gas and vapour in the pore spaces of *soils* (3.10)

[SOURCE: ISO 11074:2015, 2.1.13]

3.13
soil material
excavated soil, dredged materials and *soil* (3.10) treated to remove or destroy or reduce the environmental availability of *contaminants* (3.2)

[SOURCE: ISO 11074:2015, 7.4.16, modified — “materials composed of” removed.]

3.14
soil pores
part of the soil volume, between the solid particles of the *soil* (3.10)

[SOURCE: ISO 11074:2015, 2.1.14]

3.15
soil water
all water of the *unsaturated zone* (3.17)

[SOURCE: ISO 11074:2015, 3.2.7, modified — “and saturated” has been removed.]

3.16
total organic carbon
TOC
all carbon present in organic matter

[SOURCE: ISO 11074:2015, 2.1.22]

3.17
unsaturated zone
part of an *aquifer* (3.1) in which the pore spaces of the formation are not totally filled with water

[SOURCE: ISO 6107-2:2006, 150]

4 General

Soils are of central importance within the water cycle because their storage and filter functions have a lasting influence on the water balance and groundwater quality. In this context, particular attention shall be paid to the following functions:

- mechanical filter functions (retention of suspended sludge and contaminant particles);
- chemical filter functions (sorption and mobilization of substances);
- transformation functions (degradation or transformation of substances).

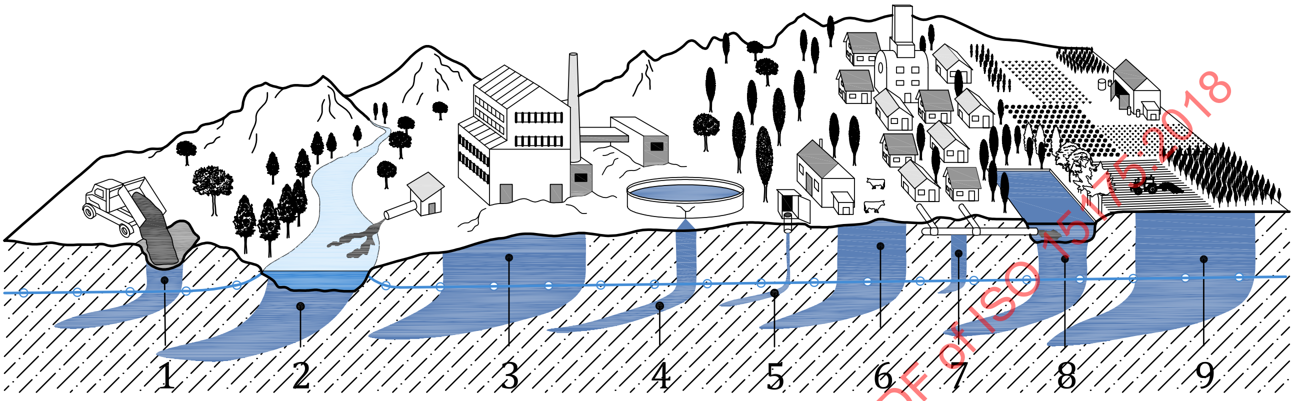
NOTE The liquid phase most commonly consists of solely of water but non-aqueous liquids can sometimes also be present as a separate phase.

Soil is understood as a porous medium consisting of three phases: the solid phase, the liquid phase and the gaseous phase. The ratio of these phases and their respective compositions vary widely in time and space.

The assessment of contamination affecting groundwater quality requires a profound understanding of the governing processes and reactions of potentially toxic compounds in soils. Contaminants are translocated in all three phases of soils as a function of the properties of the chemicals and the soil. Hence, strategies for assessing risks to groundwater due to soil contamination should vary with the contaminants considered, and should take into account those soil properties which mainly govern the soil's filter, retention, release and transformation functions.

Vaporous contaminants, essentially volatile organic compounds (VOCs) are likely to migrate in the unsaturated zone in gaseous form. Knowledge of the soil gas quality in the unsaturated zone allows detection of contamination before it reaches the saturated zone as well as in the saturated zone.

In addition to considering the properties of the chemicals and the soil governing the behaviour of contaminants in soils, different ways for contaminants to enter soils should also be evaluated when designing suitable risk assessment strategies, with respect to contamination of groundwater. Soil and groundwater contamination can be caused by different sources on different spatial scales, as indicated in Figure 1.



Key

1	solid waste tip of landfill
2	industrially-polluted “losing” river
3	industrial site drainage
4	leaking storage tanks
5	*in-situ* sanitation
6	farmyard drainage
7	leaking sewers
8	wastewater lagoons
9	agricultural intensification

Figure 1 — Common sources of groundwater contamination (focus on contaminated land management)[1]

On regional and larger scales, soil contamination is caused, for example, by wet and dry atmospheric deposition. The contamination observed in these cases is generally diffuse and with fairly moderate levels of contamination. On a local scale, a variety of point sources can cause all kinds and magnitudes of soil and groundwater contamination. In the case of immiscible contaminants (for example hydrocarbons), most of the contamination forms a separate liquid phase from water. A fraction is soluble and capable of migrating to groundwater. In the unsaturated zone, another fraction could be in the vapour phase. Depending on the relative density in water, the behaviour of the contaminant is very different. Light non aqueous phase liquids (LNAPL) have a lower density and dense non aqueous phase liquids (DNAPL) have a higher density than that of water. Most point sources of contamination can also be regarded as off-site diffuse sources of groundwater contamination. It is evident that different contamination scenarios as a function of contamination sources and scale demand different investigation strategies with respect to groundwater impact. Furthermore, groundwater impact assessment depends on the aquifer system: unconfined or confined and the type of porosity: porous media, fractured media or karst environment. At present there are no uniform principles for the investigation and evaluation of contaminated soils and contaminated sites in relation to the protection of water resources.

Investigation strategies may be simple to complex. Simple or qualitative approaches mostly refer to assessment of, for example, the potential leaching risk of chemicals through the soil towards groundwater. In contrast to complex or quantitative approaches, the level of actual soil contamination is not taken into account. Approaches of this type can also be used, for example, to classify larger areas with respect to their capability of protecting groundwater resources against contamination, or as an introductory step in an assessment of an actual contaminated site.

To assess the on-site impact on groundwater resulting from specific soil contamination, quantitative approaches based on site-specific investigation procedures including laboratory and/or field measurements have to be used. Laboratory measurements can include physical, chemical and biological analysis, and leaching tests. Assessments of this kind should also take into account natural background concentrations of a substance and other natural conditions affecting the impact on the groundwater. Assessments of impact on groundwater often include a temporal aspect, since the actual impact might not be measurable at the time of the investigation, but could happen sometime in the future.

Assessments also depend on the purposes of investigations, for example:

- conservation of soil functions in order to prevent groundwater contamination;
- soil and groundwater monitoring;
- risk assessment;
- controlling remediation measures.

A listing of suitable methods is provided in the main part of this document (see Clause 5).

Since the impact on groundwater can lead to impact on surface waters, this aspect can in some cases be relevant in an overall impact assessment. This issue is not addressed explicitly in this document.

5 Assessment of direct and indirect inputs to groundwater

5.1 General

A prerequisite for the evaluation of the soil-to-groundwater pathway is the determination of the relevant physical, chemical and biological characteristics of soils and the hydrological characteristics of the site. It is therefore necessary to collect data for the assessment of the contamination source with respect to the type and degree of contamination and extent of source(s).

It is also necessary to describe the soil that is impacted by the contamination source, and the factors affecting the impact on the groundwater, e.g. the geometry, hydraulic conditions and natural chemical and biologic processes. Indeed, many processes occurring in the soil (physical, chemical and biological processes) may influence the groundwater impact.

The processes involved are illustrated schematically in Figure 2 and a description of the relevant parameters is given in Table 1.

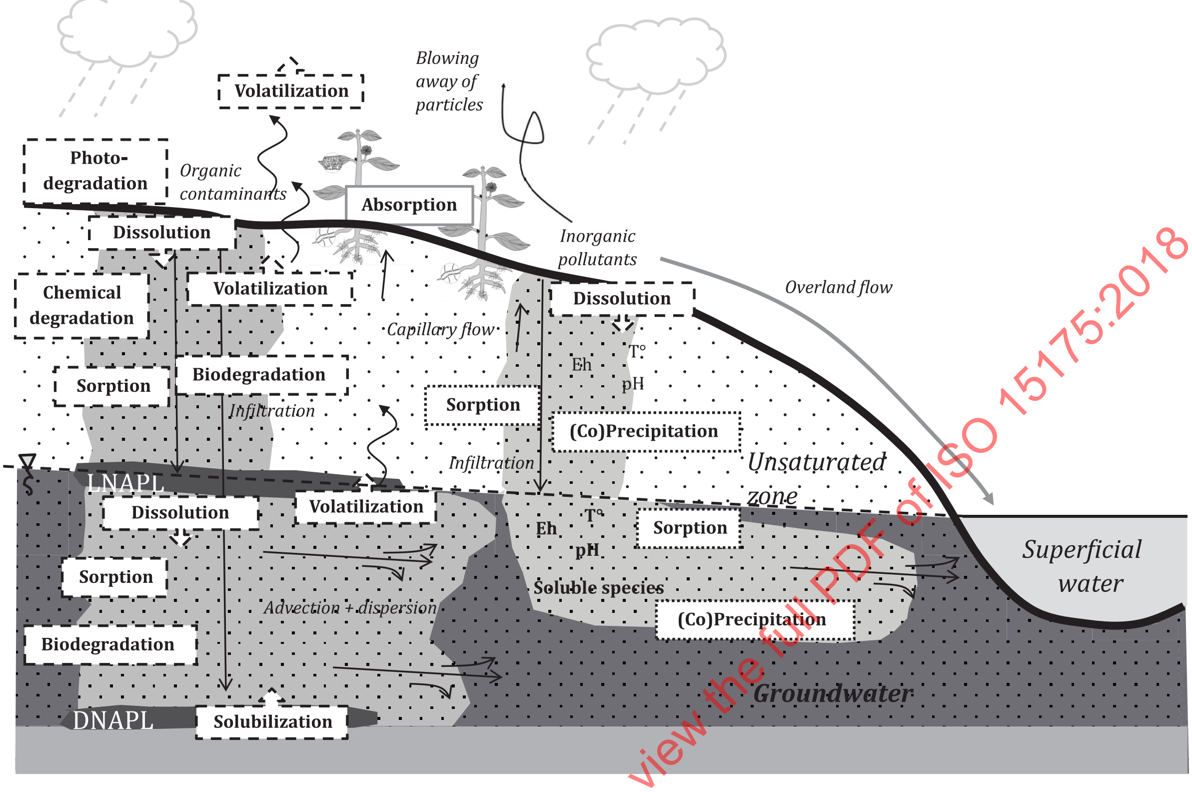


Figure 2 — Schematic diagram illustrating the soil compartment covered by the assessment procedure and processes affecting the impact of contamination on groundwater[2]

The types of information needed to describe the relevant soil compartment include pedology (e.g. soil unit), lithology of parent material, hydrogeology (e.g. permeability), physico-chemical conditions (e.g. pH) and biological conditions (e.g. substrate availability). The study area of the impact assessment depends on many factors, such as the following:

- the origin of the contamination: diffuse versus point source;
- the type and characteristics of contaminants (e.g. solubility, persistence);
- the type (e.g. consolidated, unconsolidated, sedimentary/metamorphic/igneous, fractured, karstic, dual porosity, etc.) and characteristics of the aquifer (e.g. homogeneous/heterogeneous, isotropic/anisotropic, bedding, jointing, confinement, dispersivity, velocity, etc.);
- the use of the aquifer (e.g. drinking water supply, industrial supply) and relations of the aquifer with superficial water (e.g. lakes, rivers, etc.).

5.2 Relevant soil processes

Contaminant transport in the unsaturated zone is governed not only by the transport of percolating water but also by a number of biological, physical and chemical processes. Which of these processes are to be considered important within a given context depends on the type of contaminants and the actual soil conditions. An overview of soil and contaminant parameters related to contaminant transport is given in Table 1.

Contamination ageing influences different processes in soil: decrease of degradation and mobility, increase of sorption and viscosity. This parameter should be taken into account for the impact assessment.

Table 1 — Examples of soil and contaminant parameters related to different processes in soil

Process	Examples of soil parameters	Examples of contaminant parameters
Mass transport of contaminants	Hydraulic, conductivity, degree of saturation, porosity, pore size distribution, soil water-retention functions, relative permeability, residual saturation, wettability, surface tension, capillary pressure, tortuosity	Solubility, volatility, density, viscosity Adsorption/sorption
Contaminant transport in water:		
Advection	Pressure gradient, hydraulic conductivity, porosity	
Dispersion/diffusion	Dispersitivity, pore water velocity	Diffusion coefficient
Density transport	Pore water velocity, soil layering Viscosity Dispersion, change in density	Liquid density
Preferential flow	Pore size distribution, fissure size, macropore size, connectivity Dispersion, change in density	Viscosity, density, diffusion coefficient
Volatilization	Water content, temperature, chemical-phase content	Vapour pressure, Henry's constant
Gas-phase transport	Water content, tortuosity, pressure differences	Diffusion coefficient
Dissolution of organics	Hydraulic conductivity, tortuosity, water content	Solubility, composition of chemical phase
Dissolution of inorganics	Hydraulic conductivity, tortuosity, water content	Solubility products
Precipitation	pH, redox, other components, water content	Solubility product, complexation constant
Complexation	pH, ligand concentration, dissolved organic compound DOC	Stability constant of complexes
Ion exchange	Cation exchange capacity, ionic strength, other cations, pH	Valence, degree of hydratization
Sorption of organics	pH, organic matter content, clay content and mineralogy, specific surface area	Octanol/water distribution coefficient, sorption coefficient
Sorption of inorganics	pH, organic matter content, clay content and mineralogy, specific surface area, non-crystalline (short-range ordered) oxide and hydrous oxide gels	Sorption coefficient
Degradation		
Abiotic	Redox, pH, temperature	Presence of primary susbtrate, degradability, toxicity to microorganisms
Biotic	Microorganisms, redox, substrate, pH, temperature, water content	

5.3 Impact assessment procedures

In order to complete a description of the source and the soil, it is necessary to develop:

— strategies for evaluation of site-specific parameters;

— sampling strategies;

- analytical and testing strategies;
- for each site and/or media (soil, groundwater, soil gas) that influences the impact on the groundwater.

These strategies should be determined on the basis of:

- history of the site or area;
- available data and/or results of previous investigations;
- the nature of any process-based treatment methods that have been applied to the soil;
- the intended use of the site.

To optimize the actual need for information in relation to the costs and time demanded for the investigations in the field and laboratory, the assessment should be carried out following a tiered approach (see Figure 3 which displays a generic approach which can be amended when necessary). The impact assessment is often an iterative procedure, each tier being a more refined version of the description of the problem and each leading to a more detailed basis for decision-making, as to the necessity of remedial action in the form of site clean-up, land-use restrictions, etc. (see Tier 2 on Figure 3).

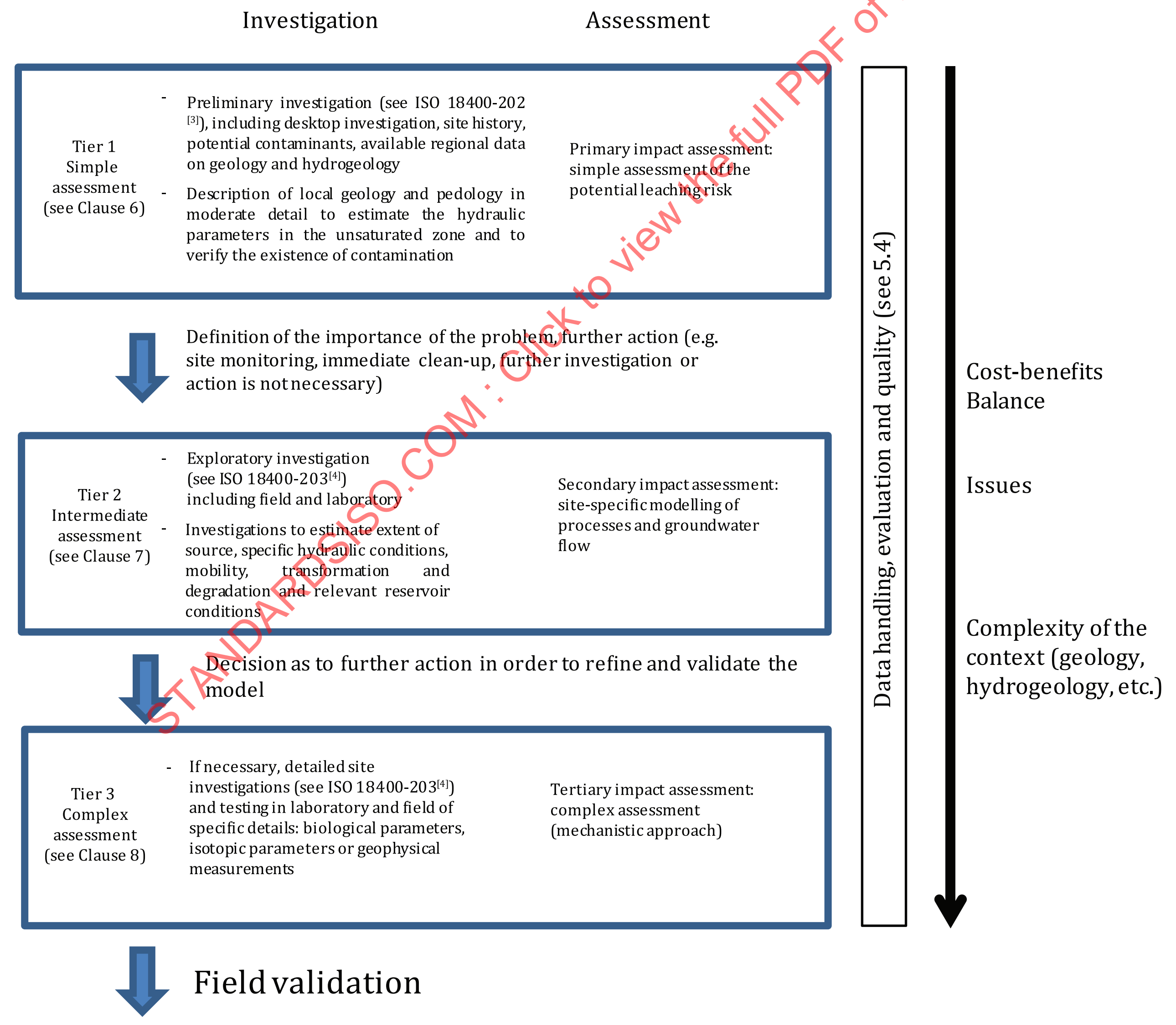


Figure 3 — Graduated approach for impact assessment

Investigations of contaminated sites are usually only carried out where contamination is expected. Thus, guidance given in ISO 18400-203[4] can be used. The area of interest may provide elements forming a basis for decision-making and for determining if a site should be remediated.

The first tier requires a preliminary investigation (desk study and site reconnaissance) (see Clause 6), such as collecting information about known or suspected contamination hot-spots and the range of expected contaminants. In the first tier, the assessment identifies presence of potential source-pathway-receptor linkages.

If this proves inconclusive, it could be necessary to locate contamination hot-spots via a targeted exploratory investigation (Tier 2). This should include the determination of total and pseudo-total concentrations of substances. If evidence of increased concentrations of contaminants can be deduced from the orientated investigations, then pathway-specific investigations are necessary. The risk of groundwater contamination in the saturated zone can, in general, be derived from the concentration and amount of substances in water in the unsaturated zone (e.g. infiltration, capillary, perched). In some cases, it may be more important to consider the amounts of contaminants instead of the concentrations, which may be very high in a small spot, without posing a large risk of groundwater contamination.

Evaluation of the exposure pathway of soil to groundwater within the framework of a second-tier risk assessment requires evaluation of the concentration of substances in the percolation water which enter the groundwater.

Within the framework of a detailed investigation, it may be necessary to consider, in addition, the volumes of transferable substances, potentially mobile fractions and other parameters.

The assessment of a groundwater contamination risk resulting from soil contamination can be performed at different levels of complexity. The more data available, the more processes can be taken into account in a risk assessment model. An example procedure is given in Annex B.

NOTE Often, the reports presenting the results of assessments are scrutinized by regulators and other interested parties, including the general public. It is important, therefore, that such reports are of a high technical standard but also take into account the diverse and often non-technical readership. Therefore, tabular summaries, graphical and other means can be used to present the data in ways that make the data and conclusions as easy as is practicable to assimilate and assess.

5.4 Sensitivity and uncertainty analysis, data handling and quality

The purpose of characterizing soil (or other media) as suggested in this document is usually to enable site assessment with respect to impact on groundwater. This document provides guidance on the types of data that might be required in an assessment, and indicates for which parameters or procedures there are international or national standards available. The assessor shall choose those parameters that are appropriate to the task in hand.

Estimations of uncertainty are of crucial importance to risk assessments, as they provide a measure of confidence in the site investigation data and ultimately the final outcome of the risk assessment. Uncertainties typically concern:

- the extent to which the contaminant data from single samples are spatially representative of the site conditions;
- the extent to which sampling techniques are adequate to ensure that a sample is representative of the site conditions at the point where it was taken;
- the extent to which analytical data reflects the actual characteristics (concentrations, form/state, mobility, etc.) of the contaminants present;
- the extent to which the pedological, geological, hydrogeological conditions at the site are understood;
- the ways in which the contaminants may behave in the environmental setting of the site and surrounding areas (fate and transport issues);

- the extent to which behaviour of the receptors potentially at risk under the particular circumstances can affect the risk estimates;
- how the receptors can be affected by the contaminants, and what role the different receptor characteristics play in this.

A sensitivity and uncertainties analysis should be conducted on each parameter to determine its influence on the results of the simulations and predictions settings. Furthermore, this analysis allows us to understand the contribution to the overall uncertainty of each parameter tested.

The model is validated by comparing the results of the predictive simulation and measurements in the field. The construction and calibration of a model are validated iteratively by comparing the results of measurements and simulation results.

Uncertainty accompanying an estimate of, for example, concentrations of contaminants in percolation water can originate from various sources. Generally, sources of uncertainty can be differentiated between knowledge or informational uncertainty and natural variability. Natural variability as a property of nature cannot be reduced while informational uncertainty can to some extent be counteracted by increased sampling or measurement efforts. Informational uncertainty can be due to uncertain data quality, such as measurement errors or incomplete data, or due to uncertain model structure and parameters. Uncertainty in model structure is the result of simplifications, assumptions or errors in the formulation of the model. Model uncertainty can also result from uncertainty in the model parameters produced in the course of model fitting.

For the problem of contaminants percolating from soils to groundwater, it is important to recognize that the processes forming the soil are physical, chemical and biological and obey physicochemical laws in a highly nonlinear way. Technically, all variations of contaminant concentrations in the percolating water are deterministic in the sense that they are a result of soil characteristics governing relevant sorption, decay or other processes. However the sensitivity of these processes to small variations in governing soil properties produces some random error, which in turn leads to undeterminable variations in the dissolved phase. Random error causes stochastic uncertainty leading to imprecision, while uncertainty in model structure (leading the model to incorrectly reproduce the process in question) causes deterministic uncertainty leading to inaccuracy.

Before any judgement can be made about impact on groundwater, the sufficiency of data on soil, soil gas and groundwater to be used should be evaluated. The data shall be sufficient in terms of:

- type;
- quantity;
- analytical/testing quality.

In the context of data quality, it is essential to:

- define the objectives of the investigation;
- establish a sampling strategy;
- establish an analytical and testing strategy taking into account the guidance in this document and other relevant International Standards;
- set data quality objectives consistent with the assessment procedure to be used.

NOTE Guidance on sampling strategies for soil quality is given in, for example, ISO 18400-104[5], for soil gas in, for example, ISO 18400-204[5] and for groundwater in, for example, ISO 5667-11[7].

It is essential to have sufficient data. The confidence that can be attached to any judgements made if no greater than the confidence there is in the representativeness of the data. For example, confidence following a site-specific risk assessment or through comparison with the requirements of authoritative guidance such as generic assessment criteria or environmental quality standards. The requirements of such guidance regarding sampling shall always be followed.

The assessor needs to bear in mind the disproportionate costs and time delays that can result if it is necessary to carry out an additional sampling exercise if, for example, a particular parameter is not determined when the opportunity is available.

Care shall be taken in deciding what statistical expression(s) of the data are to be used in the assessment, as this may affect the choice of sampling procedures. For groundwater impact investigations, a statistic such as the “95 % upper confidence level of the mean” or the “maximum observed value” is recommended (See Reference [8]).

The quality of the data to be used shall be ensured by some or all of the following:

- setting formal data quality objectives (e.g. for accuracy, reproducibility, etc.);
- using standardized analytical and testing methods such as those listed in this document or, where International Standard methods are not available, those published by national standardization or equivalent bodies;
- using laboratories using methods accredited under regional schemes.

6 Tier 1 — Simple assessment

6.1 General

The first tier includes preliminary investigations as defined, for example, in ISO 18400-202[3] based on desktop investigations and site reconnaissance with the aim of carrying out an initial impact assessment. This tier includes delineation of the soil geometry, soil unit and hydrological conditions on the basis of general knowledge of the area, possibly supplemented with some field data concerning local conditions. Specific hydraulic parameters (e.g. hydraulic conductivity, water retention characteristics and infiltration rate) can also be estimated from relevant literature (pedo-transfer functions and/or databases). The presence of contaminants and other substances of interest (e.g. possible presence of naturally occurring substances that might leach) and their likely concentrations are estimated on basis of site history and any available analyses of soil and water samples and/or soil-gas measurements. The relevant transport and decomposition processes are approximated from data related to the relevant soil conditions and contaminants retrieved from the literature. The mobility of inorganic contaminants can be estimated by assessing the soil/water partition coefficient (K_d) (see Reference [9]). For organic compounds, the soil organic carbon-water partitioning coefficient (K_{oc}) should be estimated preferably with passive sampling given in References [10] and [11].

Relevant parameters required for the physical and chemical characterization are listed in Annex A together with suitable methods for their determination or evaluation.

If the Tier 1 assessment indicates a need for a more detailed assessment, the Tier 2 assessment should be carried out. The relevant investigations consisting of sampling, chemical analysis and field tests are planned on the basis of Tier 1.

6.2 Site and soil description

The assessment of the potential impacts of contaminated soil on groundwater requires general information about the site under investigation. The most relevant parameters for a site-description are listed in Table 2. For example, ISO 18400-202[3] could be applied. The scale at which this information may be collected, and the degree of detail that is required, is closely related to the objective of the investigation which primarily depends on the anticipated nature and distribution of contamination (see ISO 18400-203[4]). During a desktop investigation (Tier 1 according to Figure 3), gathering information about the site does not include field work, whereas further investigation tiers may necessitate more detailed field data collection. It is important to bear in mind that the reliability of data interpretation and risk assessment strongly depends on a profound knowledge of the site under consideration, hence collection of information about the parameters listed in Table 2 should be as comprehensive as possible.

Table 2 — Examples of parameters for site and soil description

Parameters		Applicable International Standard
Landform and topography	Topography, landform, land element, position, slope, micro-topography	ISO 25177[12] ISO 18400-202[3]
Land use and vegetation	Land use, human influence, vegetation	
Geology and lithology	Kind of parent material, effective soil depth	
Surface characteristics	Soil outcrops, surface coarse fragments, erosion phenomena, surface sealing, surface cracks, other characteristics	
Soil-water relationship	Surface water balance, rainfall, evapotranspiration, groundwater recharge, presence and depth of water table(s), site drainage, moisture conditions	
Soil type/soil profile description	Soil unit in regards of the classification system used Sequence and depth of diagnostic horizons, kind of boundaries Soil colour (matrix, mottling) Organic matter Texture, coarse elements, presence of non-soil material Carbonates, field-pH, electrical conductivity Structure, voids, fracturing, inhomogeneities Compactness and consistence Total estimated porosity Roots, worm channels, biological activity	

6.3 Simple assessment of the potential leaching risk

The application of simple assessment models is recommended specifically for:

- landscape management purposes (e.g. definition of drinking-water protection zones, environmental impact studies on regional and larger scales);
- evaluation of the potential and actual contamination of soil to the groundwater from inorganic and organic contaminants [e.g. fertilisers (nutrients like nitrogen), plant treatments (pesticides), treatments of sewage sludge, compost or other organic waste material (heavy metals, organic compounds)].

Simple assessments only need a very limited number of easily available input data, but are consequently restricted in their assessment to relative evaluations. Mostly they are applied in order to classify the soil's inherent binding force and leaching risk, preferably on a regional or larger scale, when quantitative information about the actual soil contamination is lacking.

Simple assessment methods can be characterized as deterministic approaches with a modular structure. They are based on simple empirical relations using mathematically derived and formalized matrices, and thus they rigorously simplify the underlying physical and/or chemical processes. In contrast to complex assessment models (see Annex B), the relevant transport and transformation phenomena in soils are not described on a process-orientated basis. Simple assessment approaches are often categorized as "functional" or "non-mechanistic" models which consist of pedotransfer functions and rules (see Reference [13]). With respect to water and solute fluxes, they refer at least to the principle of mass balance.

Functional forecasting models aim at relative evaluations, for example in terms of a low, medium or high leaching risk. The result of a qualitative risk assessment is expressed as a potential leaching risk because, in contrast to quantitative "mechanistic" models (see Annex B), the actual soil contamination is not taken into account. The physical, chemical and biological properties (see Clause 5) of the soil and its contaminants are generally needed as input data. The information on soil properties is available from soil maps and digital soil information systems, or can be derived from them by applying simple transfer rules and transfer functions (see Reference [14]). Additionally, information on climate, hydrology and land use is also often provided in digital information systems or from paper maps.

The application of simple assessment models is restricted to moderately contaminated soils, whereas complex evaluations are carried out in case of strong suspicion of soil contamination predominantly on a local scale. With respect to the kind and limited number of input data and the level of risk evaluation, simple assessment models might not be an adequate substitute for site-specific investigations (i.e. laboratory and/or field measurements in order to quantitatively evaluate assumed or ascertained soil contamination) as suggested in Annex B). Simple assessment models should not be used for evaluation of spill situations or concentrated input from a point source. Nevertheless, a simple risk assessment might be a helpful introductory tier in an assessment of an actual contaminated site.

7 Tier 2 — Intermediate assessment

7.1 General

Tier 2 typically includes sampling and analysis or testing to estimate the extent of the source(s), and the distribution of contaminants in the soil matrix between the different phases: the soil gas, within or bound to the soil particles, or dissolved in the soil water (see e.g. ISO 18400-203[4]). The transport of contaminants in various soil types and underlying lithologies (e.g. sand versus fractured rock) can be very different depending on their static and dynamic characteristics. It is very important in Tier 2 to determine the dominant mechanism(s) governing various processes. For example, if the transport is mainly through fractures in clay and rock, then the adsorption process can be of minor importance. Alternatively, in homogeneous sand with a high organic matter content, adsorption can be the most important process to take into account in the impact assessment. Information about the groundwater reservoir (e.g. extent, importance for the water supply) in question is also relevant in this phase in order to be able to assess the severity of a potential problem. Leaching and extraction tests can be applied to assess the distribution of contaminants between the soil, water and geochemical phases, and to assess the potential environmental impact (on groundwater in this context) and possible remediation actions required. The seasonal pattern of climatic characteristics should be known in order to evaluate seasonal trends in potential and ongoing soil and groundwater contamination. Management practices should also be taken into account (e.g. irrigation type and quantities). Site-specific computer modelling of processes and groundwater flow can also be introduced as part of this tier. In Tier 2, quantitative methods as exemplified in Table B.7 can be useful.

7.2 Sampling

Before starting any investigation, it is essential to define the objectives of the investigation and to prepare a sampling strategy consistent with those objectives (see, for example, ISO 18400-104[5] and ISO 18400-203[4]). Reference should be made to relevant International Standards and to the guidance attached to any national criteria or standards relating to soil quality that are to be used in the assessment of the results of the investigation. In some jurisdictions, there could be a legal requirement to follow certain procedures if published criteria are to be used as the basis of the assessment.

Different sampling procedures could be required for contamination due to different sources. International ISO standard may be applied for each considered sources. Otherwise, appropriate national standards or equivalent regulations should be used.

7.3 Characterization of soil, water and soil gas

7.3.1 General

The description and assessment of contaminated sites require information on soil, soil gas and water characteristics. In Annex A, relevant parameters required for the physical, chemical and biological characterization of soil, water and soil gas are listed.

The principles that should govern strategies for determination of relevant analysis and tests are provided in 5.2 and 5.3. Examples of the application of such procedures in the context of assessment methods are provided in Annex B. Qualitative or simple assessment approaches (see 7.1) require, in addition to the general site and soil description (see Table 2), selected physical (see Table A.1) and basic chemical parameters (see Table A.2) as input data. Tables A.3, A.4 and A.5 list international standards that might be applicable for relevant inorganic and organic contaminants[29]-[115].

More complex assessment methods mostly require an extended and more specific data input, in particular with respect to the actual concentrations of potential contaminants in soils and water.

7.3.2 Physical parameters

A number of soil physical parameters are relevant in connection with the assessment of groundwater and contaminant transport in the unsaturated zone (see Table A.1). The actual choice of parameters measured should be based on preliminary knowledge of site characteristics and the contaminant situation (Tier 1). Table A.1 lists International Standards that might be applicable[29]-[115].

In order to estimate hydraulic data for the saturated zone (e.g. hydraulic conductivity, transmissivity, leakage, etc.) pumping tests can be carried out. With this type of test, groundwater flow in the saturated zone can be described. Water migration in the unsaturated zone can be estimated on the basis of measurements of grain size distribution (e.g. by pedo-transfer functions/rules). However, inhomogeneities can dominate the distribution and velocity of the infiltration. If more accurate estimates are necessary, infiltration tests can be performed on site.

7.3.3 Chemical parameters

7.3.3.1 General

Conventionally, the chemical parameters to be measured are grouped as follows:

- basic characteristic parameters (see Table A.2);
- inorganic nutrients (see Table A.3);
- inorganic contaminants (see Table A.4);
- organic contaminants (see Table A.5).

In many cases, it can be useful to apply leaching/extraction tests to provide information about the release of specified contaminants under reference conditions, or under conditions that more closely approximate or simulate the actual field situation under consideration. Leaching/extraction tests cover a range of experimental procedures and systems, from simple one soil-sample/one-extractant systems (e.g. strong acid, weak extractant/complexing agents and water) to more sophisticated column-flow systems. Commonly, all tests or extractions result in an eluate/leachant that should be analysed for basic parameters, inorganic and/or organic contaminants with the analytical methods described in this subclause.

Any test needs to be validated to confirm the test method will not result in loss of the organic contaminant (e.g. via loss of volatiles in preparation stage or losses due to the filtering by adsorption to the filtering equipment).

It is important that the contaminant situation in the soil, both in the source zone and at the water table, are well described. The choice of parameters depends on the actual site history and the specific aim of the investigation. It should be noted that the choice of method influences the actual concentration measured, and the assessor should ascertain which methods are the most appropriate for different types of assessment.

Before any laboratory analysis, samples should be subjected to pretreatment (e.g. ground, sub sampled) compatible with the method(s) of analysis to be employed. Some methods for extraction or analysis include their own requirements regarding pretreatment of samples and these shall always be followed unless there are sound technical reasons not to do so, in which case those reasons should be reported with the analytical results.

A number of so-called basic characteristic parameters (see Table A.2) influence soil processes that affect contaminant concentrations, e.g. adsorption, precipitation and complexation.

7.3.3.2 Inorganic substances

Nutrients (see Table A.3) can be of importance both in themselves and/or as necessary constituents for the biological degradation of organic compounds. The International Standards listed in Table A.3 can be applied.

Metals and metalloids (see Table A.4) can be naturally occurring or present as contaminants that at higher concentrations might become pollutants. Table A.4 lists International Standards that might be applicable to their determination.

7.3.3.3 Organic substances

While the inorganic analyst is primarily concerned with the analysis of a defined number of elements and anions, the organic analyst is often interested in looking for any organic compound which might be present. In practice, organic analyses take two forms:

- determination of what is present (qualitative analysis);
- determination of how much of a specific compound or class of compounds is present (quantitative analysis).

The detection of "adventitious" or unexpected substances, particularly when complex mixtures of organic chemical species are present, requires the use of analytical screening methods, such as gas chromatography/mass spectrometry. It is also customary to employ analytical methods that purport to give total concentrations of classes of compounds such as phenols, polycyclic aromatic hydrocarbons (PAHs), total petroleum hydrocarbons (TPH) and chlorinated hydrocarbons. Care is required in both the use and interpretation of the results of such methods. Qualitative analysis is frequently carried out prior to quantitative analysis. Class analyses frequently precede specific compound analyses.

"Total" applied to organic compounds usually means that an analytical technique has been employed that cannot distinguish between similar compounds: e.g. in the case of phenols between monohydric, dihydric and trihydric compounds (i.e. compounds with one, two and three hydroxyl groups attached to the benzene ring). However, the term "total" may be misleading: perhaps not all phenols can be detected by the method employed (e.g. there may be limitations in terms of molar mass or the number and size of other functional groups present on the benzene ring) and different methods can give different results.

Many organic analyses involve extraction with an organic solvent. The solvent used and the conditions of extraction can influence the analytical results. For example, volatile PAHs (generally those of lower molar mass) may be lost during a hot Soxhlet-style extraction, whereas a cold extraction may be less effective in dissolving higher molar mass PAHs. This might be important, for example, when trying to determine residual concentrations of PAHs in a soil material subjected to thermal treatment, those remaining might be expected to be those less volatile.

Analyses of soil materials for volatile organic compounds (e.g. benzene, chlorinated solvents) present particular analytical difficulties. Research suggests that even under ideal conditions of sampling, transport and sample preparation, substantial losses can occur (one study suggested that 50 % retention was the best that could be achieved). Under less than ideal conditions, almost all can be lost (see Reference [15]). Some guidance on how to overcome these problems is given in ISO 18512[16] and ISO 22155[17].

NOTE To limit the loss of volatile organic compounds, the soil sample can be stored in methanol as soon as it is collected in the field.

The use of *in situ* methods, such as soil vapour analysis, are likely to give a more reliable indication of distribution and relative concentrations of the substances of concern. In addition, it should be noted that different laboratory methods (e.g. purge-and-trap and head-space analysis) can give substantially different results.

It is important to recognize that organic compounds can be extracted from naturally occurring organic materials (e.g. organic matter, decaying vegetation, peat, coal) and that non-specific analyses, in particular can, therefore, give misleading results.

Table A.5 lists International Standards that might be applicable for organic contaminants that are the more commonly encountered, but the list is not exhaustive[29]-[115].

7.4 Impact assessment

7.4.1 General

Predictive modelling of the behaviour of inorganic or organic substances in soils with respect to the resulting leaching risk to groundwater can be used to assess impacts for sites that are considered of particular importance because of their complexity and/or potentially severe impact on groundwater resources.

The choice of the model depends on the context, the conceptual model (geology and hydrogeology of the site), the type of contaminant, the quality and availability of information and the limits of the transport model (scope). It is important to note that the complexity of the model should be adapted to suit the properties of the field of study. In addition, the model selected shall be representative of the studied system and shall contribute to the assessment and final decision. The objects and advantages of the model shall be clearly defined before use.

7.4.2 Substance concentration in soil water

7.4.2.1 General

For the estimation of concentrations of substances in percolation water, any of the following approaches can be used:

- estimation of concentrations in soil water based on groundwater investigations.
- direct investigation of soil water.

7.4.2.2 Estimation of concentrations in soil water based on soil investigations

To avoid problems caused in the direct investigation of concentrations of soil water, investigation of the contaminated soil matrix can be undertaken (e.g. batch methods). This requires methods which are as accurate as possible to confirm the natural soil solid/solution ratio.

The methods given in Table A.4, which describe mobile/mobilizable contents of heavy metals and other trace elements (complexing/weak extractant/water soluble), have a greater liquid/solid ratio in the presence of complexing agents. Therefore, concentrations determined on this basis (e.g. leaching tests) tend to overestimate the real content of trace substances in soil percolation water.

In addition to the above-mentioned batch methods, the soil solution can also be obtained by using column tests. These methods are especially applicable for organic contaminants.

Where leaching tests are used, ISO 18772[18] is followed as a logical process to facilitate the selection and justification of appropriate tests based on a conceptual understanding of soil and contaminant properties, likely and worst-case exposure conditions, leaching mechanisms, and study objectives.

During risk assessment, one should characterize the leaching behaviour of contaminated soils using an appropriate suite of tests. As a minimum, these tests should be:

- upflow percolation column test, run to LS 2 — to derive kappa values;
- pH dependence test if pH shifts are realistically predicted with regard to soil properties and exposure scenario;
- LS 2 batch test — to benchmark results of a simple compliance test against the final step of the column test.

7.4.2.3 Estimation of the concentrations of substances in soil water based on groundwater investigations

Under constant conditions and known volumes of percolation water and groundwater flow, the concentrations in the soil water can be estimated from concentrations in the groundwater by following the hydraulic gradient downstream from the location of contamination.

The relevant data needed to draw a conclusion can only be obtained if the hydrogeological site conditions are not too complex. Moreover, this method is usually not sufficient to provide the local differentiation necessary for selection and design of remediation measures.

7.4.2.4 Direct investigation of soil water

The direct investigation of concentrations in percolation water requires sampling of soil percolation water by suitable means, e.g. suction devices to obtain soil water *in situ*. Soil water samplers, also called suction lysimeters, can be used to collect water samples in the soil profile. The samplers are installed at the desired depth and left in the soil, allowing periodic sampling to occur with minimal disturbance of the soil. The samplers consist basically of a porous ceramic cup and a sample collection tube. A vacuum pump is used to create a vacuum in the sampler, which draws water from the soil matrix through the ceramic cup and into the sampler. The water sample can then be extracted from the collection tube and taken to the lab for chemical analysis.

Application of this method can encounter the following problems:

- insufficient water to be sampled from the unsaturated zone;
- sorption effects, depending on the material of the device used;
- undefined spatial zone sampled by the method;
- high sampling frequency required to evaluate efforts to determine variability of the soil and concentrations of substances.

7.4.3 Amount of transferable substances

To evaluate the risk of groundwater contamination, it might be necessary to determine substance amounts (volumes and/or masses) entering the groundwater. Therefore, it is necessary to consider not only the concentration of substances, but also the volume of percolation water and the relevant soil area. Firstly, the net infiltration rate, averaged over one year, can be determined as climatic water balance. The relevant site parameters are given in Table 2.

NOTE Climatic water balance characterizes the concurrent availability of energy and water for biota and is represented here by actual evapotranspiration and climatic water deficit.

Depending on the specific site conditions and the substances under consideration, infiltration rate may not be sufficient and it may be necessary to quantify the flux of water through the soil and the corresponding substance concentrations at a higher resolution with respect to aspects of time and space by carrying out site specific investigations.

7.4.4 Degradation of organic contaminants

For organic contaminants, (bio)degradation should be taken into account when extrapolating from a given substance concentration in the unsaturated zone to a substance concentration in the upper aquifer. Biodegradation may occur as part of the natural attenuation processes in the unsaturated zone. Due consideration should be given to the conceptual site model and its potential for biodegradation to occur. If suitable data are not available, additional substance-specific degradation experiments could be necessary.

8 Tier 3 — Complex assessment

8.1 General

If the assessment still has to be improved after Tier 2, supplementary tiers can be carried out. The content of these following tiers can consist of some of the same elements as in Tier 2, but with improved accuracy of information available, e.g. by taking more samples to determine the influence of heterogeneity in the soil. Supplemental sorption, degradation and leaching tests can be carried out in the laboratory with conditions taking into account the evolution of the site (variations of pH, redox potential, etc.). The form of the contaminant-bearing solid phases can also be assessed with laboratory methods [e.g. X-ray diffraction (XRD), scanning electron microscopy coupled with energy dispersive X-ray (SEM/EDX) spectroscopy, extended X-ray absorption fine structure (EXAFS)].

The use of other tools such as biological parameters (8.2), isotopic parameters (8.3) or geophysical parameters (8.4) can be useful in order to refine the quantitative assessment.

In Tier 3, quantitative methods as exemplified in Annex B can be useful.

It can be seen that the assessment is often an iterative procedure, each tier being a more refined version of the description of the problem and each leading to a more detailed basis for decision-making, as to the necessity of remedial action in the form of site clean-up, land-use restrictions, etc.

8.2 Biological parameters

Biological parameters are often of specific interest for groundwater contamination risk assessment because they influence:

— degradability of organic compounds in soils: the contaminant concentration at the water table depends not only on dilution and adsorption but also on the microbial influence on degradable components. To be able to assess this activity in both the present and future situation, information on the microbial activity (see Table A.6) in the soil in question is important;

— (eco)toxicological potential of organic compounds in the percolating soil water or groundwater: if the evaluation of soil contamination aims at determining the leachability and/or bioavailability and/or biodisponibility of organic compounds, eco-toxicological investigations of the liquid phase (see Table A.6) can be carried out to characterize the soil's inherent retention capacity analogously to physical and chemical extraction or leaching tests (see ISO 21268 series[9]).

The biological parameters that might be relevant are listed in Table A.6 together with International Standards that can be used[29]-[115].

8.3 Isotopic parameters

Isotopic tools can give information about the hydrogeological characteristics and, in particular, the determination of the flow lines, the definition of the recharge area, the estimated transfer time or residence time of water, the existence of one or more aquifers and possible connectivity between these systems, and the influence of surface water (see References [19], [20] and [21]). For this, the stable isotopes of the water molecule (δ^2H and $\delta^{18}O$), radioactive isotopes, methods for dating waters (CFCs,

SF_6, 3H, ^{14}C, $^{3}He/^{3}H$, ^{222}Rn) and tools developed specifically for other applications such as the origin of contaminants ($^{87}Sr/^{86}Sr$, $\delta^{11}B$, $\delta^{34}S$ and $\delta^{18}O$ of SO_4) are used as well as artificial tracers (Table A.7).

Characterization of a contaminated site with reliable answers about the origin and fate of organic contaminants in environmental media is often difficult to achieve with conventional investigation methods. Isotopic analysis of individual organic compounds (compound-specific isotope analysis — CSIA) offers a quick and tangible mean to obtain additional information on *in situ* processes.

CSIA can give a quick answer to differentiate reduction in concentrations due evaporation, dispersion or dilution from a net loss of contaminants due to biotic and/or abiotic transformation. A change in isotopic ratios of a contaminant from its source to the hydraulic piezometers downstream reveals that this contaminant has been processed. CSIA can provide tangible evidence of the presence of *in situ* biodegradation of contaminants as the isotopic composition (e.g. $\delta^{13}C$) is changing differently according to the processes.

Isotopic analyses can be an additional tool “2nd-line-of-evidence” for providing strong evidence of degradation (in the absence of solid evidence offered by conventional chemical and microbial testing, for example) and to distinguish the original contaminants or metabolites (differentiate an initial metabolite degradation product).

8.4 Geophysical parameters

Geophysical methods can be used at different stages of a study of contaminated sites and soils in order to:

- improve the geological and hydrogeological model;
- make the environmental diagnosis of a site in order to identify potential sources and plumes;
- monitoring a plume on:
  - its geometry;
  - changes in concentration of the contaminant;
  - changes in physicochemical properties of the contaminant, related to redox reactions (particularly changes in the redox potential).

Unlike conventional monitoring techniques using analysis of soil or water from boreholes, geophysical methods are inclusive, non-destructive and can be continuous in time.

Annex A
(informative)

Relevant parameters suggested for the physical, chemical and biological characterization of soil, water and soil gas

Table A.1 — Physical parameters

Parameter	Methods			Soil[a]	Water[a]	Soil gas	Applicable International Standard[b]
	Tier 1	Tier 2	Tier 3				
Texture	sieving, sedimentation			X			ISO 11277 (s)
Coarse material	sieving			X			ISO 11277 (s)
Presence of non-soil material	Sieving Visual inspection			X			ISO 25177(s)
Hydraulic conductivity (unsaturated and/or saturated)	literature (pedotransfer functions, databases)	laboratory and field methods (e.g. Guelph constant- head permeameter, Darcy test, wind's evaporation)		X			ISO 11275 ISO 17313 ISO 22282-4 (s)
Temperature	temperature sensors			X	X	X	
Water-retention characteristics	literature (pedotransfer functions, databases)	stepwise extraction of water by suction or tension		X			ISO 11274 (s)
Soil water content (ex situ)	gravimetric methods neutron depth probe, TDR (Time Domain Reflectometry)			X			ISO 16586 (s) ISO 11465 (s) ISO 10573(s)
Pore size distribution	estimation from soil water-retention curves			X			ISO 25177(s)
Field capacity	estimation from soil water-retention curves			X			ISO 11274(s)
Bulk density	direct measurement on undisturbed soil samples, estimation from soil water retention curves			X			ISO 11272(s)
Infiltration rate	Literature (parameters for site and soil description — see 5.4)	constant head pressure infiltrometer		X			ISO 22282-5
Atmospheric pressure						X	

[a] "X" indicates that the information or characteristic could be relevant. However, decisions should always be made on a case-specific basis.

[b] If available, (s) standard method for soil, (w) for water and (g) for gas.

Table A.2 — Chemical parameters — Basic characteristic parameters

Parameter	Tier 1	Tier 2	Tier 3	Soil[a]	Water[a]	Applicable International Standard[b]
pH	pH-electrode			X	X	ISO 10390 (s) ISO 10523 (w)
Redox potential	Redox electrode			X	X	ISO 11271 (s)
TOC (Total Organic Carbon)	Combustion Sulfochromic oxidation			X	X	ISO 10694(s) ISO 14235(s) ISO 8245(w)
DOC (Dissolved Organic Carbon)	Combustion after filtering (0,45 µm)			X	X	ISO 14235 (s) ISO 8245(w)
Organic carbon	Dry combustion, sulfochromic oxidation				X	ISO 10694(s)
Carbonate content	CO_2-evolution			X	X	ISO 10693 (s)
Specific electrical conductivity	EC-meter			X	X	ISO 11265 (s) ISO 7888 (w)
Cation exchange capacity		$BaCl_2$ unbuffered, $BaCl_2$ buffered at pH 8,1		X X		ISO 11260 (s) ISO 13536 (s)
Exchangeable acidity		Titration of barium chloride extracts		X		ISO 14254 (s)
Elemental composition	On site measurement by energy-dispersive X-ray fluorescence			X		ISO 13196 ISO 18227 EN 15309
Contaminant-bearing solid phase			Laboratory methods (X-ray diffraction [XRD], scanning electron microscopy coupled with Energy Dispersive X-ray (SEM/EDX) Spectroscopy, Extended X-ray absorption fine structure (EXAFS), etc.]	X		
Soil/Water partition coefficient (K_d)	Literature (databases). K_d can also be estimated from Kow	Laboratory methods (batch and column leaching test)		X		ISO 21268 (all parts)

[a] "X" indicates that the information or characteristic could be relevant. However, decisions about relevance should always be made on a case-specific basis.

[b] If available, (s) standard method for soil, (w) standard method for water.

Table A.3 — Nutrient contaminants

Nutrient, for example	Specification/form	Extraction methods	Soil[a]	Water[a]	Applicable International Standard[b]
Calcium				X	ISO 7980 (w) ISO 14911 (w) ISO 11885 (w)
Magnesium				X	ISO 7980 (w) ISO 14911 (w) ISO 11885 (w)
Sodium	Water soluble	H_2O		X	ISO 9964-1 (w) ISO 9964-3 (w) ISO 14911 (w) ISO 11885 (w)
Potassium	Water soluble	H_2O		X X	ISO 9964-2 (w) ISO 9964-3 (w) ISO 11885 (w)
	Water soluble	H_2O	X	X	ISO 14911 (w)
Nitrogen	Total	Dry combustion (modified) Kjeldahl Peroxodisulfate oxidation	X X	X	ISO 13878 (s) ISO 11261 (s) ISO 11905-1 (w)
	Nitrate	$CaCl_2$-extraction, dry soils KCl-extraction, moist soils sulfosalicylic acid	X	X	ISO 14255 (s) ISO 14256-2 (s) ISO 7890-3 (w)
	Ammonium	$CaCl_2$-extraction, dry soils KCl-extraction, moist soils	X X	X	ISO 14255 (s) ISO 14256-2 (s) ISO 7150-1 (w)
	Water soluble	$CaCl_2$-extraction, dry soils	X		ISO 14255 (s)
Phosphorus	Total	Aqua regia		X	ISO 6878 (w) ISO 11885 (w)
	Weak extractant	Na(HCO_3)-extraction	X		ISO 11263 (s)
Sulfur	Total	Dry combustion, aqua regia	X		ISO 15178 (s) ISO 11885 (w)
	Weak extractant	Dilute HCl	X		ISO 11048 (s)
	Water soluble	H_2O	X		ISO 11048 (s)

[a] "X" indicates the information or characteristic could be relevant. However, decisions about relevance should always be made on a case-specific basis.

[b] If available, (s) standard method for soil, (w) standard method for water.

Table A.4 — Inorganic contaminants — Metals, metalloids, trace elements

Metals, metalloids and trace elements[a] for example	Specification/form	Extraction/preparation method	Soil[b]	Water[b]	Applicable International Standard[c]	
					Extracted/preparation method	Determination method
Arsenic Barium Cadmium Chromium Cobalt Copper Cyanides Iron Lead Manganese Mercury[d] Molybdenum Nickel Selenium Thallium Zinc	total	Alkaline fusion	X		ISO 14869-2 (s)	ISO 22036 (s) ISO 11047 (s) ISO 20279 (s) (Thallium only) ISO 11047 (s) ISO 20280 (s) (Arsenic, Selenium)
		HF + $HClO_4$	X		ISO 14869-1 (s)	
	Pseudo-total	Acid mixture of nitric acid (HNO_3), hydrofluoric acid (HF) and hydrochloric acid (HCl)	X		ISO 14869-3 (s)	
		Aqua regia	X		ISO 11466 (s) ISO 20279 (s) (Thallium only) ISO 11047 (s) ISO 20280 (s) (Arsenic, Selenium) ISO 16772 (s) (Mercury only)	
	Complexing	EDTA buffered DTPA	X		ISO 14870 (s)	
	Weak extractant	Diluted acids (e.g. HNO_3)	X			
		$NaNO_3$	X			
		NH_4NO_3	X			
		$CaCl_2$	X			
		KCl	X			
		H_2O	X		See NOTE	See NOTE

NOTE There are a variety of extraction and analytical methods for soil and soil-water in the series of International Standards which might be applicable. However, it is important to confirm that they work with the extracts obtained from a particular (often contaminated) soil material.

[a] Can be potentially harmful at higher concentrations.

[b] "X" indicates that the information or characteristic could be relevant. However, decisions about relevance should always be made on a case-specific basis.

[c] If available, (s) standard for soil.

[d] Mercury can be also analysed in soil gas.

Table A.5 — Organic contaminants

Substance/groups of substances	Speciation	Methods	Soil[a]	Water[a]	Soil gas	Applicable International Standard[b]
petroleum hydrocarbons	Gasoline	GC/FID	X	X		ISO 16703
	Diesel		X	X		ISO 11423-1 (w)
				X		ISO 11423-2 (w)
	Hydrocarbons (C10-C40)	GC/FID or GC-MS Purge and trap thermodersorption TPHCWG		X	X	ISO 15009 (s) ISO 16703 ISO 15009 (w) ISO TS 16558-2 (s)
	Volatiles componds (C6-C10)	GC/ECD		X	X	ISO 15009 (s)
		Purge and trap thermodesorption		X		ISO 10301 (w) ISO 22155 (s)
		GC/ECD or head space technique				ISO 16558-1 (s)
Water-miscible solvents (e.g. ethanol, methanol, MTBE, ETBE)				X		ISO 22854 (W) ISO 22155 (W)
perfluorooctanesulfonate (PFOS)				X		ISO 25101 (w)
PAHs	e.g. EPA-16	Soxhlet/HPLC/UV RP C-18/HPLC	X	X		ISO 7981-2 (w) ISO 17993 (w) ISO 28540 (w) ISO 18287 (s)
Phthalates			X	X		ISO 18856 (w)
Phenols, chlorophenols		Acetone/GC/ECD	X	X		ISO 14154 (s) ISO 8165-1 (w) ISO/TS 17182 (s)
Pesticides	Phenoxys	RP C-18/HPLC/UV Immunoassay HPLC GC-MS	X	X		ISO 11369 (w) ISO 11370 (w) ISO 15089 (w) OIML R 112 (s) ISO 11264 (s) ISO 15913 (w) ISO 27108 (w) ISO/TS 28581 (w) ISO 16308 (w)

NOTE There are a variety of extraction and analytical methods for water in the series of International Standards which might be applicable. However, it is important to confirm that they work with the extracts obtained from a particular (contaminated) soil material.

[a] "X" indicates that the information or characteristic could be relevant. However, decisions about relevance should always be made on a case-specific basis.

[b] If available, (s) standard method for soil, (w) standard method for water.

Table A.5 *(continued)*

Substance/groups of substances	Speciation	Methods	Soil[a]	Water[a]	Soil gas	Applicable International Standard[b]
PCB, chlorobenzenes, organocloro pesticides		GC/ECD	X	X		ISO 10382 (s) ISO 6468 (w)
Chlorinated aliphatics	AOX	Purge and trap	X X	X X	X	ISO 15009 (s) ISO 10301 (w) ISO 22155 (s) ISO 9562 (w)
Triazines, phenylurea herbicides		HPLC	X			ISO 11264 (s) ISO 15913 (w) ISO 11369 (w)

NOTE There are a variety of extraction and analytical methods for water in the series of International Standards which might be applicable. However, it is important to confirm that they work with the extracts obtained from a particular (contaminated) soil material.

[a] “X” indicates that the information or characteristic could be relevant. However, decisions about relevance should always be made on a case-specific basis.

[b] If available, (s) standard method for soil, (w) standard method for water.

Table A.6 — Biologic parameters

General characteristic	Special measurement/example	Soil[a]	Water[a]	Applicable International Standard[b]
Microbial activity	Mineralization of organic chemicals	X		ISO 14239 (s)
	Biodegradation under aerobic conditions	X		ISO 112666 (s)
	Biodegradation under anaerobic conditions	X		ISO 15473 (s)
	Nitrogen mineralization	X		ISO 14238 (s)
Ecotoxicity	Inhibition of luminescence		X X X	ISO 11348-1 (w) ISO 11348-2 (w) ISO 11348-3 (w)
	Inhibition of biomass (algae test)		X	ISO 15799 (w)
	Inhibition of plant growth (ecotoxical effect on early growth stage)		X	
	Acute immobilization (inhibition of mobility of Daphnia)		X	ISO 6341 (w) ISO 15799 (w)
Biological pathogens		X	X	

[a] “X” indicates that the information or characteristic may be relevant. However, decisions about relevance should always be made on a case-specific basis.

[b] If available, (s) standard method for soil, (w) standard method for water.

Table A.7 — Isotopic parameters

Characteristics of aquifers	
Porosity, dispersivity, transmissivity, storage, residence time, vulnerability	^{222}Rn, artificial tracers ^{2}H,^{18}O, ^{3}H, ^{3}H-^{3}He, CFCs, ^{14}C
Quantitative parameters	
Area and recharge rates	^{2}H-^{18}O, ^{3}H, ^{3}H-^{3}He, CFCs, ^{14}C, artificial tracers
Flow	^{3}H, ^{3}H-^{3}He, ^{85}Kr, CFCs, ^{14}C, artificial tracers
Interaction of surface water - groundwater	^{2}H,^{18}O, ^{3}H, ^{222}Rn, ^{87}Sr/^{86}Sr, artificial tracers
Interactions between aquifers	^{2}H, ^{18}O, ^{3}H, ^{14}C, ^{87}Sr/^{86}Sr, artificial tracers
Groundwater quality	
Origin and source of contaminants	Isotopes of B, C, N, S, Cl
Contaminant transport	^{3}H, ^{3}H-^{3}He,, CFCs, ^{14}C, U/Th
Chemical and biological processes	isotopes of B, C, N, S

Annex B

(informative)

Examples of complex methods for assessing the leaching risk

B.1 General

The complex assessment approach (see Clause 8) can be summarized as follows:

- Step 1: Calculation of dilution in the saturated zone;
- Step 2: Calculation of dilution in the saturated zone downstream of the point source;
- Step 3: Calculation considering dispersion, adsorption and degradation phenomena in the saturated and unsaturated zone.

The unsaturated zone is considered only within step 3 (so this is not a stepwise procedure for the unsaturated zone) and without specifying how to consider it.

B.2 Dissolved substances (inorganics and organics)

B.2.1 Considering the unsaturated zone

B.2.1.1 General

Given the complexity of the unsaturated zone, the characterization of sites and the calculation of predictable impacts of the transfer of substances could be expensive and difficult in some situations.

However, a tiered method is proposed here. It includes several steps of modelling (steps 0, 1, 2 and 3), from simpler to more complex. It is illustrated in Figure B.1.

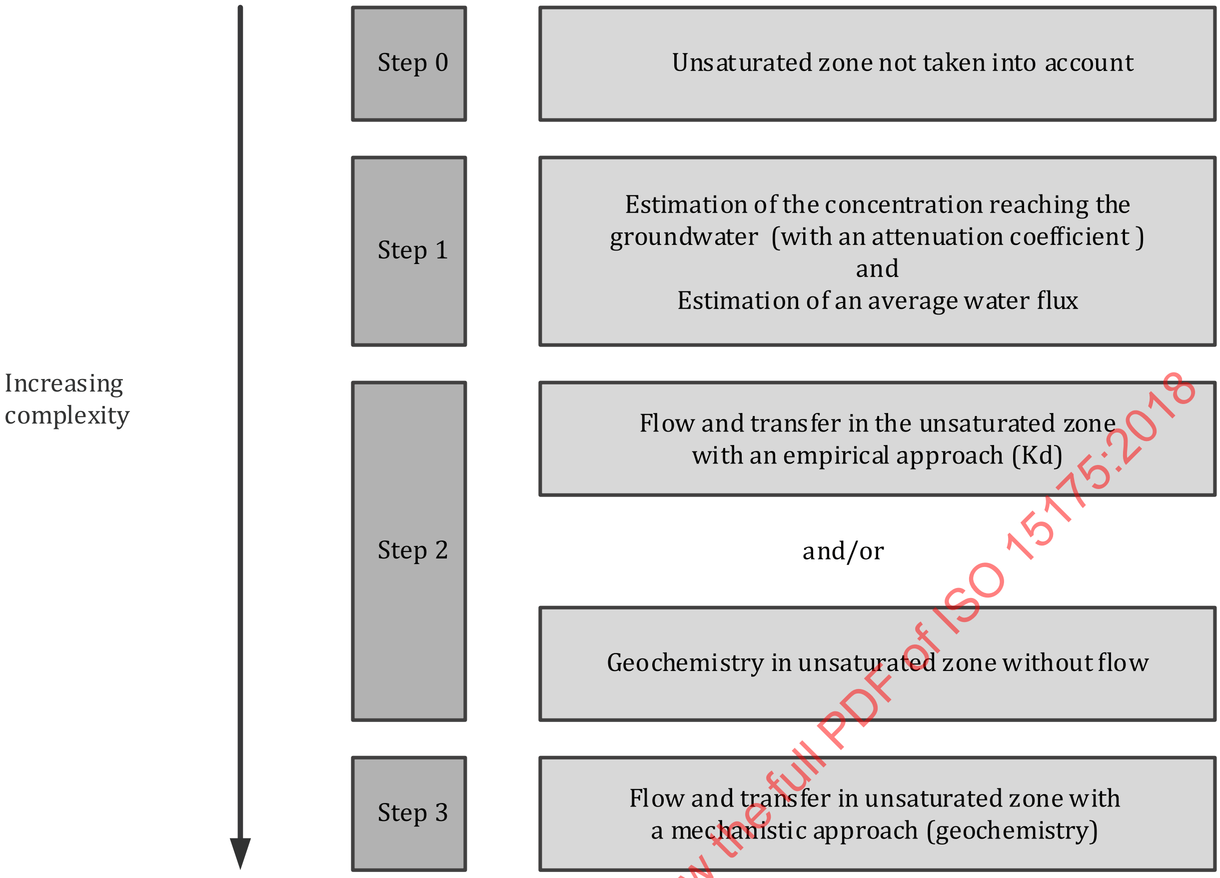


Figure B.1 — Stepwise procedure for groundwater risk assessment related to the presence of contaminants in the unsaturated zone[22]

The choice of the step depends on the following:

- a cost/benefit analysis, comparing advantages brought by the modelling of each step to human and material;
- costs related to the acquisition of parameters and modelling, and also to costs of eventual compensatory measures (recovery, containment, etc.) related to the presence of contaminants;
- the complexity of the context (geological, hydrogeological, etc.) of the site;
- the issues (economical, environmental, societal, etc.) related to the presence of contaminants in the unsaturated zone.

In the case where there is a regulatory and/or environmental constraint on the site under consideration, such as regulatory maximum concentrations that are set at a receptor (e.g. drinking water standards), the motivation to go from one step to the next can be the comparison of this maximum permitted concentration with the calculated one (from the modelling): if the calculated concentration is higher than the maximum concentration allowed, going to the next step should be considered. Even if it is more complex and more expensive to implement, it becomes more realistic and so less potentially penalizing in terms by reducing uncertainties. The steps are applied to the circumstances of the site under consideration with an increasing level of detail required by the assessor in progressing through the steps.

For all cases, when it is about quantifying the impact of the transfer of contaminants to the water resource, the consideration of the transfer in the saturated zone is essential after the step of modelling in the unsaturated zone.

B.2.1.2 Step 0

This first step does not take into account the unsaturated zone. Step 0 considers that the transfer between the ground surface and the surface of the groundwater is immediate and that the concentration in pore water, at the contaminated zone, is the same concentration reaching the saturated zone.

The pore water concentration in the contaminated area could be estimated from an analysis of the contaminated material, from a leaching or a percolation test.

This level 0 does not need any calculation.

B.2.1.3 Step 1

The mass flux of contaminant F reaching the groundwater is shown as Formula (B.1):

$$F = C_{ea} \,.\, v \tag{B.1}$$

where

F is the mass flux of contaminant ($ML^{-2}T^{-1}$);

C_{ea} is the concentration in pore water reaching the groundwater (ML^{-3});

v is the transfer velocity (LT^{-1}).

Step 1 estimates the pore water concentration C_{ea} reaching the groundwater in the same way as Step 0 but with the application of a dilution coefficient. This dilution coefficient is like an average concentration in the unsaturated zone. During its transfer through the unsaturated zone, the contaminant concentration in pore water in the contaminated zone ($C_{dissolved}$) is multiplied by a factor, given by Formula (B.2) (see Reference [23]):

$$C_{ea} = C_{dissolved} \,.\, d_{vc}/d_v \tag{B.2}$$

where

C_{ea} is the concentration in the pore water reaching the groundwater (ML^{-3});

$C_{dissolved}$ is the concentration in the pore water of the contaminated zone (ML^{-3});

d_{vc} is the thickness of the contaminated zone (L);

d_v is the total thickness of the unsaturated zone (L).

Formula (B.2) is based on the hypothesis that the source of contamination has a finite mass and considers that the concentration C_{ea} is constant, so it does not reflect the decrease of the source concentration over time.

A simple analytic solution to calculate the velocity, v, of a contaminant in the unsaturated zone is given as Formula (B.3)(see Reference [24]):

$$v = \frac{I}{\theta_v . R_f} \tag{B.3}$$

where

v is the average velocity of the contaminant in the unsaturated zone (LT^{-1});

I is the effective annual infiltration (LT^{-1});

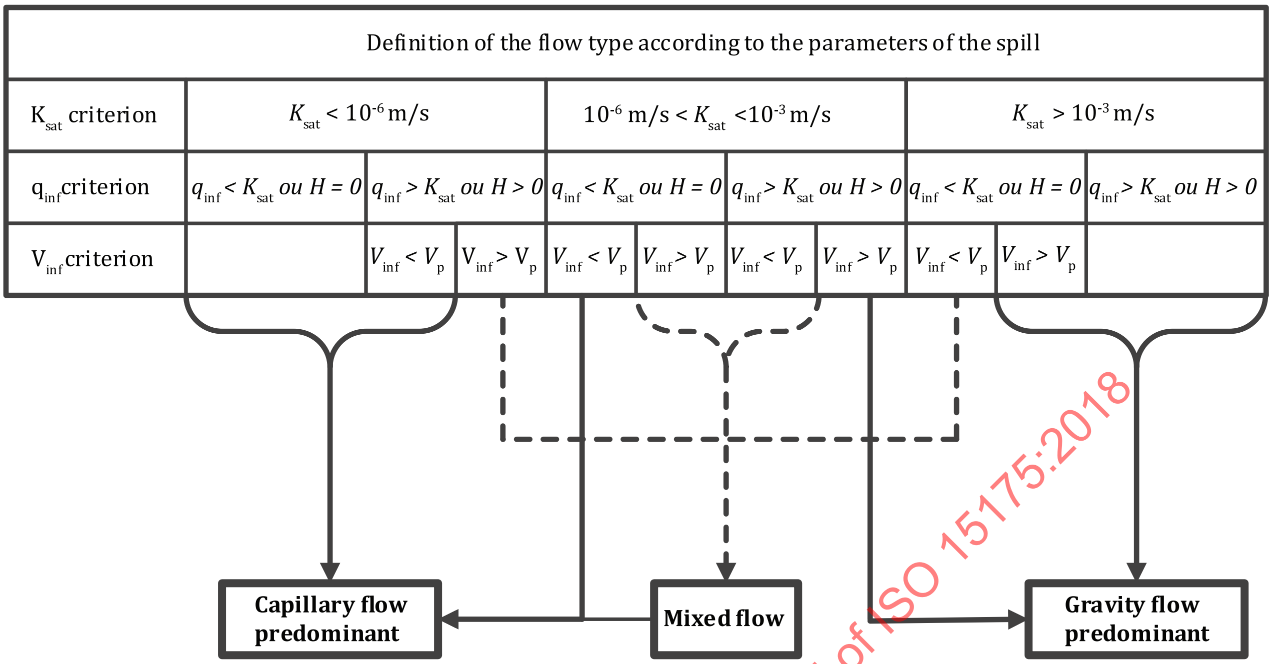
θ_v is the average volumetric water content in the unsaturated zone (–);

R_f is the lag effect (–).

Formula (B.3) is an approximation because it does not consider the variations over time of the surface infiltration or the spatial variations of the water content.

In the case where the flow is homogenous, stationary and mostly conditioned by gravity, it is possible to represent the unsaturated zone by a porous medium, totally saturated. In this case, the transfer velocity can be estimated with the Darcy equation, considering the hydraulic conductivity at saturation, a unit hydraulic gradient, an average volumetric water content and eventually a delay factor. This approximation can be done with the help of an analytic solution or a numerical model.

Figure B.2 can be used to define the conditions in which the flow is mostly conditioned by gravity.



Definition of the flow type according to the parameters of the spill										
K_{sat} criterion	$K_{sat} < 10^{-6}$ m/s			10^{-6} m/s $< K_{sat} < 10^{-3}$ m/s				$K_{sat} > 10^{-3}$ m/s		
q_{inf} criterion	$q_{inf} < K_{sat}$ ou $H = 0$	$q_{inf} > K_{sat}$ ou $H > 0$		$q_{inf} < K_{sat}$ ou $H = 0$		$q_{inf} > K_{sat}$ ou $H > 0$		$q_{inf} < K_{sat}$ ou $H = 0$		$q_{inf} > K_{sat}$ ou $H > 0$
V_{inf} criterion		$V_{inf} < V_p$	$V_{inf} > V_p$	$V_{inf} < V_p$	$V_{inf} > V_p$	$V_{inf} < V_p$	$V_{inf} > V_p$	$V_{inf} < V_p$	$V_{inf} > V_p$	

Key

K_{sat}	hydraulic conductivity
V_{inf}	volume of the infiltration
q_{inf}	infiltration velocity (defined as follows: q_{inf} approximately $V_{inf}/(T_{inf} \times S_{inf})$ with T_{inf}: duration of the infiltration and S_{inf}: area of the infiltration)
H	water pressure head
V_p	pore volume (defined as follows: V_p approximately $S_{inf} \times e_{nsz} \times \mathcal{E}$ with S_{inf}: area of the infiltration, e_{usz}: thickness of the unsaturated zone and $\mathcal{E}$: total porosity)

NOTE K_{sat} thresholds are indicative (see Reference [25]) and their use is to be discussed for each site.

Figure B.2 — Selection of methods to characterize the main flow parameters according to the flow type[26]

B.2.1.4 Step 2

- **Flow and transfer in the unsaturated zone with an empirical approach (K_d).**

  This approach is about modelling flows and transfers in the unsaturated zone. The modelling of the chemistry of the contaminant is simplified. The transfer of species is modelled considering a delay factor which considers all the physicochemical processes (adsorption, complexation, precipitation, etc.). This delay factor depends on the solid/liquid partition coefficient (K_d).

  An approach, simplifying but majoring in terms of impacts towards water resource, is about modelling a contaminant behaviour, such as the one of a tracer, that is to say such as the behaviour of a conservative substance (which does not degrade), and non-reactive (which does not react with the host environment).This is simply translated by the consideration of a K_d equal to 0.

  This step can be completed by a geochemical modelling without transfer.

- **Geochemistry without flow (or “geochemistry in batch”)**

  Especially for metallic trace elements, before making a linked “chemical-transfer” modelling (Step 3), a geochemical modelling without transfer (i.e. without spatial dimension) allows to test the purely chemical part of the model. Including chemical speciation and solubility calculation, this modelling allows to trace different graphs like:

- diagrams showing the evolution of the concentration of a metallic element according to different chemical variables (pH, Eh, etc.);
- diagrams showing predominance ranges of different phases (aqueous or solid) according to the environmental conditions (for instance diagram “Eh/pH”);
- diagrams showing the solubility variations of a solid phase according to the environmental conditions.

Associated with a sensibility study and comparing the results to the observations on site, this step allows a better comprehension of phenomena governing the environmental chemistry.

B.2.1.5 Step 3

Flow and transfer are modellised and chemistry is treated at a more detailed level with a mechanistic approach: the geochemical/transfer model allows to take into account the different mechanisms (precipitation/dissolution, surface complexation, cationic exchange, surface precipitation, co-precipitation, degradation, etc.), with a spatial and eventually a temporal (transient conditions) dimension. Using such a model needs much more time and will rather be used for sites with major issues. Moreover it needs a very good knowledge of the environmental conditions (chemistry, mineralogy and physical properties).

The model to use for this step needs two types of codes:

- a geochemical code to stimulate physico-chemical reactions;
- a transfer code to simulate the mobility of the element (diffusion/dispersion, convection).

Figure B.3 represents a flowchart which allows to identify physical functionality of the modelled case and physical types of models. Five filters are proposed:

- the flowing fluid phases;
- the contaminants;
- the non-reactive transfer models;
- the mass transfer mechanisms;
- the reactive mechanisms.

The models in this flowchart at least consider the flow in the unsaturated zone with dispersive transfer (codes without transfer are not retained, even in the case of a flow in a partially saturated environment). Neither the analytical solutions nor the geochemical codes are considered in this flowchart.