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ACCOUNTING FOR UNCERTAINTIES IN CONTAMINATED LAND MANAGEMENT

Review and Outlook

FINAL REPORT

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DISCLAIMER

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SUMMARY

ABSTRACT

On the occasion of the 4th national research meeting on contaminated land, on November 26th and 27th 2019 in Paris, ADEME called for a synthesis on uncertainties in the field of contaminated land management, including proposals for further research. This report, which has no claim to completeness given the scope of the topic, seeks to identify sources of uncertainty at different stages of the data cycle in a context of contaminated land management, to describe approaches for addressing these uncertainties and also to identify some avenues for further research.

The data cycle ranges from the sampling stage (soil, water, air, …), to using the collected information for defining site management options, through analysis, representation, interpretation, etc. While uncertainty can be generically defined as "*not being certain*", research in the past thirty years or so illustrates the importance of "*uncertainty sources*". In particular, does uncertainty relative to such and such a mechanism influencing environmental impacts and/or health risks, originate from variability related to the mechanism's random character (uncertainty of so-called "*stochastic*" origin), or rather from the incomplete and/or imprecise nature of our knowledge regarding the mechanism (uncertainty of *"epistemic*" origin)? For some authors, the confusion between these two sources of uncertainty is one of the most common shortcomings in the field of uncertainty management.

It is clear from this synthesis that while there exists no "*one-size-fits-all*" method for addressing uncertainties in a context of contaminated land management, it is possible however to promote *consistency* between the choice of uncertainty treatment methods and the nature of the information that is actually available in practice. Such an effort should promote more reliable and robust contaminated land management options. Among the different stages of the data cycle in this context, it is also important to consider communication with stakeholders. Indeed, managing uncertainties cannot rely solely on, e.g., computational approaches, but should also call on the humanities and social sciences to integrate uncertainties into a shared understanding of issues associated with contaminated land.

RÉSUMÉ

A l'occasion des 4èmes rencontres nationales de la recherche sur les sites et sols pollués, les 26 et 27 novembre 2019 à Paris, l'ADEME a souhaité une synthèse relative à la notion d'incertitude dans le domaine de la gestion des sites et sols pollués (SSP) et des propositions de pistes de recherche future. Le présent rapport, qui n'a aucune prétention d'exhaustivité compte tenu de l'étendue de la problématique, s'attache à identifier des sources d'incertitude aux différentes étapes du cycle de la donnée en contexte de SSP, à décrire des approches permettant d'appréhender ces incertitudes et à proposer des pistes de recherche.

Le cycle de la donnée considéré va de l'échantillonnage des milieux en contexte de SSP, à l'utilisation des informations collectées pour définir des choix de gestion, en passant par l'analyse, la représentation, l'interprétation, etc. Si on peut définir de manière générique l'incertitude comme étant le fait « *de ne pas être certain* », les travaux de ces trente dernières années illustrent l'importance de la notion de « *source d'incertitude* ». En particulier, le fait de ne pas être certain quant à tel ou tel phénomène influençant les impacts sur les milieux ou les risques pour la santé, dépend-il d'une variabilité liée au caractère aléatoire du phénomène (incertitude d'origine « *stochastique* »), ou alors au caractère incomplet et/ou imprécis de la connaissance que nous avons de ce phénomène (incertitude d'origine « *épistémique* ») ? Pour certains auteurs, la confusion entre ces deux sources d'incertitude constitue l'une des erreurs les plus courantes en matière de gestion des incertitudes.

Il ressort notamment de cette synthèse que s'il n'existe pas de méthode « *passe-partout* » pour gérer les incertitudes de manière générique en contexte de sites et sols pollués, on peut néanmoins promouvoir une certaine *cohérence* entre le choix des méthodes et la nature des informations dont on dispose dans la pratique. Cette recherche de cohérence devrait favoriser des choix de gestion plus fiables et robustes. Parmi les étapes du cycle de la donnée en contexte de SSP, il convient de considérer également la communication avec les parties prenantes. En effet, la gestion des incertitudes ne peut s'appuyer uniquement sur, notamment, des approches purement calculatoires, mais devrait également faire appel aux sciences humaines et sociales pour que les incertitudes soient intégrées dans une compréhension partagée des enjeux liés aux sites et sols pollués.

1. Introduction

1.1. Context and work objectives

There are scientific issues that remain relevant despite the passing of the years. The issue of uncertainties in contaminated land management is one such example. Already discussed at the first edition of the French national research meetings on contaminated land, organized by ADEME on December 12th and 13th 2002, this issue is still an important research topic that ADEME wished to address again during the 4th meeting, on November 26th and 27th 2019.

As these meetings aim to take stock of recent achievements in the management of contaminated land, but also to identify research needs and transfer of research results to operators in the field, ADEME asked for summary presentations that shed light on the current state of knowledge and open up prospects for further research. Given the scope of the problem, this synthesis on uncertainties in contaminated land management does not have any claim to completeness. Moreover, the content of this synthesis is strongly influenced by the previous work of its authors.

Among the concepts underlying this document is the idea, which emerged over the past 30 years, that the way we represent information and associated uncertainty should be consistent with the nature of the data that is actually available. Indeed, while uncertainty can be pragmatically defined as "not being certain", **what is most important with respect to uncertainties are the "sources of uncertainty", the nature of which may differ, as well as their consequences in terms of contaminated land management.** Particular emphasis is therefore placed on the sources of uncertainty that appear at the various stages of the information cycle (environmental data) in a context of contaminated land management.

1.2. The data cycle in contaminated land management

Lord Kelvin (1824 - 1907) allegedly said: "*If you can't measure it, you can't improve it*." This maxim also applies to contaminated land management, where measurement holds a special place in view of the variety of parameters that can influence the mobility and fate of pollutants, as well as the associated exposures and impacts, depending on the nature of these pollutants but also on the various matrixes impacted (soils, water, soil gas, plants, etc.).

As a contaminated site is prone to significant changes over time, the acquisition of data for management purposes is not necessarily a linear process, with a beginning and an end, but rather an iterative process, with several steps. This is illustrated schematically in **Figure 1**, which refers to the French national methodology for contaminated land management (DGPR, 2017). For a given state of the environment and further to historical and documentary studies, the investigator will define a sampling strategy and then carry out the actual sampling. The sample is prepared for analysis, and the results are represented and interpreted. Then come the stages of consultation and communication with various stakeholders, the use of the results to justify management options (evacuation of contaminated land, in situ remediation, etc.) and their use in a context of site monitoring or for the collection of new data. The entire cycle is subject to a data storage effort in order to preserve the memory of the site's environmental condition.

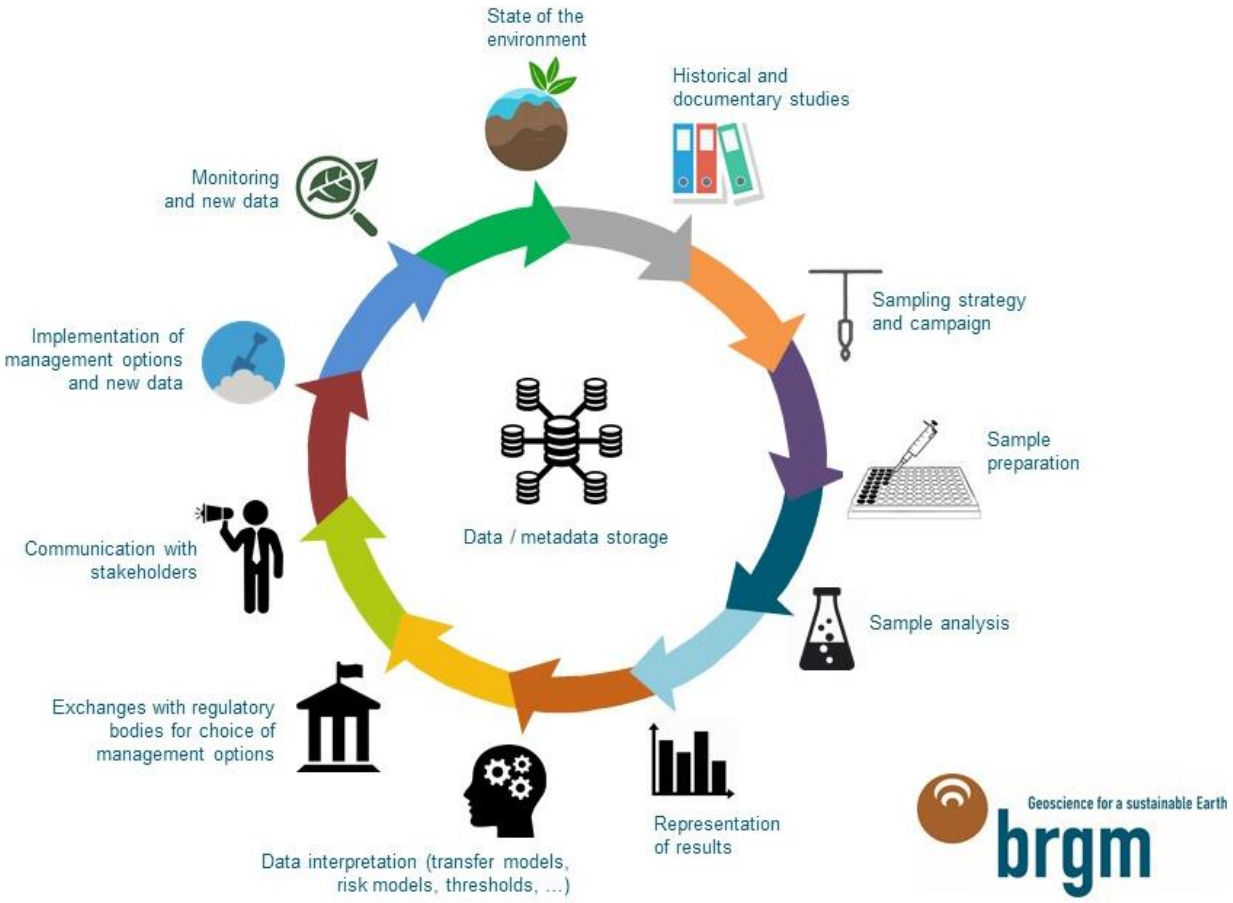

Figure 1 - Cycle of environmental data in a context of contaminated land management.

Each stage of this cycle either generates uncertainty, or is affected by sources of uncertainty. In the following, these steps are addressed by highlighting recent results and questions, with an aim to underline scope for further research.

1.3. The notion of uncertainty in the history of science

The concern to formalize the notion of uncertainty mainly goes back to the 17th century, with the contributions of Pascal, Fermat, and Huygens with respect to gambling and how to share the expected gains among players (Hacking, 1975). This is the birth of probability theory. However, from the very beginning, this notion has a dual nature. Indeed: one either models the frequencies observed in a game of chance after repeated trials, or one evaluates the degree of belief of an individual in the occurrence of an event or the truth of a proposition (as illustrated by Pascal's bet). In the first case, a random phenomenon is objectively modelled and the term “chance” is used. The term "probability," as an attribute of opinion, is used in the second case. Bernoulli then looked at both aspects, although he is best known for proving the law of large numbers, which pertains to the so-called frequentist version of probabilities. This law establishes that the empirical average, calculated on the values of a sample, converges towards the mathematical expectation when the sample size goes to infinity.

Applied primarily to gambling (random phenomena), the developed indicators of probability are unique indicators, as opposed to imprecise probabilities in the case of a so-called epistemic origin of uncertainty (related to the incomplete and/or imprecise nature of available information) and discussed in section 2.4 with particular emphasis on the theory of belief functions (Shafer, 1976). But as Shafer's article (1978) has shown, Bernoulli already set some milestones by considering the problem of merging independent

uncertain testimonies, for which he does not assume that the sum of probabilities (and not chances) of contrary propositions is equal to 1. The additivity of degrees of belief is not as natural as that of frequency-based objective probabilities. The additive vision of epistemic probabilities results from a deterministic view of the world (current in that time) which leads to consider that one can list situations of equal possibility and assume them to be equi-probable (according to the so-called principle of insufficient reason). For example, Laplace considered using such non-frequentist probabilities.

The interest in the calculus of non-additive probabilities and in the problem of merging testimonies faded in the 18th century (except for works such as Lambert's, published in 1764; see Shafer, 1978), due to the development of “hard sciences”, and then of statistics in the 19th century. The 20th century witnessed both the mathematical foundations of probability theory, derived from statistics (thus frequentist) with the work of Kolmogorov and, in parallel, the (re)birth of subjective probabilities with the work of Ramsey (1926) and De Finetti (1937), for whom "probability does not exist". In the latter case, an operational definition of subjective probabilities as additive degrees of belief is provided, considering that the subjective probability of an event is measured by the price an individual agrees to pay to buy or sell a lottery ticket that yields one euro to the buyer if the event occurs. In this context, any non-additive degree of belief is irrational as it leads to a sure loss of money. Note that the use of a gain of one euro in this reasoning has the advantage that the price that the player is willing to pay is directly equated with a subjective probability value.

This probabilistic representation of degree of belief based on exchangeable bets was endorsed in economics as part of Leonard Savage's decision theory in the early 1950s (Savage, 1954). He proposed assumptions of rationality governing the order of preference between decisions whose outcome depends on the unknown state of the world. If these assumptions are respected, the uncertainty of the decision-maker may be represented by a subjective measure of probability and the possible decisions classified according to the mathematical expectation of the utility of their consequences. This criterion of expected usefulness is formally identical to that proposed by Von Neumann and Morgenstern (1953) when the frequencies of occurrence of world states are known.

Savage's result helped establish subjective probability as an ideal tool to represent belief, even when statistical information on frequencies is missing or decision is not repeatable. But decision theory based on additive probabilities was undermined by the empirical tests of Ellsberg, who in the 1960s showed that, as a whole, individuals subjected to choices in the presence of partial ignorance (successive draws from an urn whose composition is not known) do not follow the criterion of expected utility in the sense of a single subjective probability, but adopt a cautious attitude towards incomplete information (Ellsberg, 1961). This has led to a whole literature in which incomplete information from decision-makers is modelled by more general functions than probabilities and decision criteria are of the "Choquet integral" type (Chateauneuf and Cohen, 2009).

Subjective probabilities underlie so-called Bayesian methods (Gelman et al., 2003), where one chooses to model prior expectations at the beginning of a learning process using single probability distributions, even if it leads to revise these first judgments by assigning increasingly lower weights to the prior assumptions as new observations become available. This revision is carried out using the Bayes theorem (1763), known as the conditional probability theorem.

In artificial intelligence, the same trend as in economics has been observed since the 1970s for the modelling of uncertainty in areas such as for example the formalization of reasoning under uncertainty, or the fusion of uncertain information. Three theories have emerged to address the uncertainty caused by incomplete information, namely, in order of increasing generality:

- Possibility theory (Dubois and Prade, 1988), originally conceived by Zadeh, to represent linguistic information pertaining to numerical quantities using fuzzy sets (Zadeh, 1978). More generally, the representation of expert information in the form of nested confidence intervals takes the form of possibility distributions;
- Dempster-Shafer's theory of belief functions (Shafer, 1976), which assigns probabilities not to states of the world, but to states of knowledge about the world (we no longer give the probability that a fact is true or false, but also assign a weight to the possibility of ignorance). In this case, the sum of the degrees of belief in a fact and its opposite is no longer equal to 1. It may be less than 1, and even 0 (in case of ignorance). This setting, which includes probability as a special case, allows us to represent uncertain testimonies as well as statistics with incomplete observations;

- Peter Walley's theory of imprecise probabilities, which takes up the notion of subjective probability measured by the prices of gambles, but without the requirement that selling prices must be equal to purchase prices (Walley, 1991). The use of families of probability measures is then justified from which upper and lower probabilities are extracted. This framework also captures the case of incompletely specified probabilistic models (see Augustine et al., 2014).

These approaches make it possible to distinguish between uncertainty of epistemic versus stochastic origin, a distinction that already prevailed at the beginning of the history of probabilities. This expanded framework for uncertain information poses new problems for the elicitation and the propagation of uncertainty. The existence of these formal frameworks, which are increasingly accepted for the representation of the uncertain and which differ mainly in their level of mathematical generality, encourage to revisit risk analysis methods because, instead of representing everything by single probability distributions, representation must be chosen according to the nature and quality of the information obtained by the experts or by the available observations. The idea is to stick to the available information as best as possible without arbitrarily adding any. Moreover, when some expert supplies uncertain information, we must understand whether it expresses ill-known frequencies, or pure degrees of belief? How to manage the difference between frequency (repeatable events) and belief (unique events)? A discussion is provided in Flage et al. (2016).

1.4. Recent developments regarding uncertainties related to contaminated land management

1.4.1. Current practice in contaminated land management

The French national methodology for managing contaminated land (DGPR, 2017), lists several types of uncertainty: from sampling, analyses, etc., but does not recommend methods for addressing these uncertainties and their consequences in terms of management options. It does consider, however, the quantitative assessment of uncertainties in the case of the spatial analyses of parameter distributions (e.g. pollutant concentrations), using the kriging method (Chilès and Delfiner, 1999; see section 2.4.8).

In assessing the environmental and/or health risks associated with contaminated land, a common practice in an operational setting (e.g., a consulting company) is to estimate, often by expert judgment, plausible ranges of values for the parameters influencing risk, and then to estimate [min, max] bounds for risk, based on the parameter bounds. There is at least one significant drawback to this approach. When comparing the estimated risk to a threshold, assumed here to be "accurate" (see section 2.4.6) and assuming that [min, max] risk bounds have been rigorously identified (by scanning over all possible parameter values), three situations illustrated in **Figure 2** can be distinguished. If the maximum estimated risk is below the acceptable risk threshold (**Figure 2a**), then it can be concluded that the estimated risk is acceptable. If, on the contrary, the threshold is below the min value of the estimated risk (**Figure 2b**), then the risk is unacceptable. Ambiguity appears in the most common situation where the risk threshold is somewhere between the min and max limits of the estimated risk (**Figure 2c**). In this case one cannot conclude, as there is no discrimination of evidence within the [min, max] risk interval (unlike the case of a single probability distribution for example).

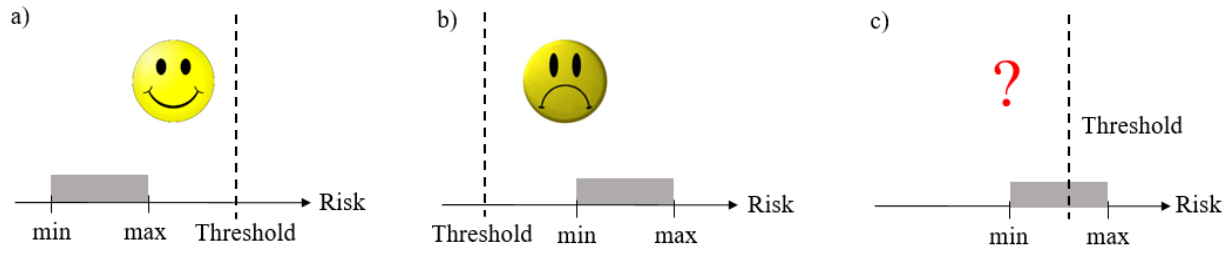

Figure 2 - Three situations comparing a [min, max] risk interval to a risk threshold

To address this problem, some recommend defining probability distributions by applying a so-called "maximum entropy" principle (Cover and Thomas, 2006) in reference to a "Bayesian" framework, and so-called subjective probability distributions: since information on probability distributions for some of the

parameters influencing risk is not available, let us assume the simplest distribution; i.e., the uniform distribution. But this approach has the disadvantage of being non-conservative, as it tends to artificially minimize the range of estimated risk, promoting estimates close to average values.

The problem is schematically illustrated in **Figure 3**. Let us assume we have a "risk model," noted C, which results from the sum of two risk factors noted A and B and that we are interested in the average value of C. All we know about A is that it is located somewhere between 0 and 1, while B is somewhere between 1 and 2. Applying a simple interval calculation (**Figure 3a**) it is deduced that C is located somewhere between 1 and 3, but we cannot express any preference within this interval and therefore in this case one cannot identify an average value. If now it is assumed that A and B are represented by uniform probability distributions on the same supports as the previous intervals (**Figure 3b**), then the sum of A and B is a triangular probability distribution of mode 2 and support [1-3]. In this case the average value is equal to the mode, i.e. 2. It can therefore be seen that the assumption of uniform distributions provides an accurate value of the average, but this precision may be illusory if the hypothesis of uniform distributions is not justified by the available information.

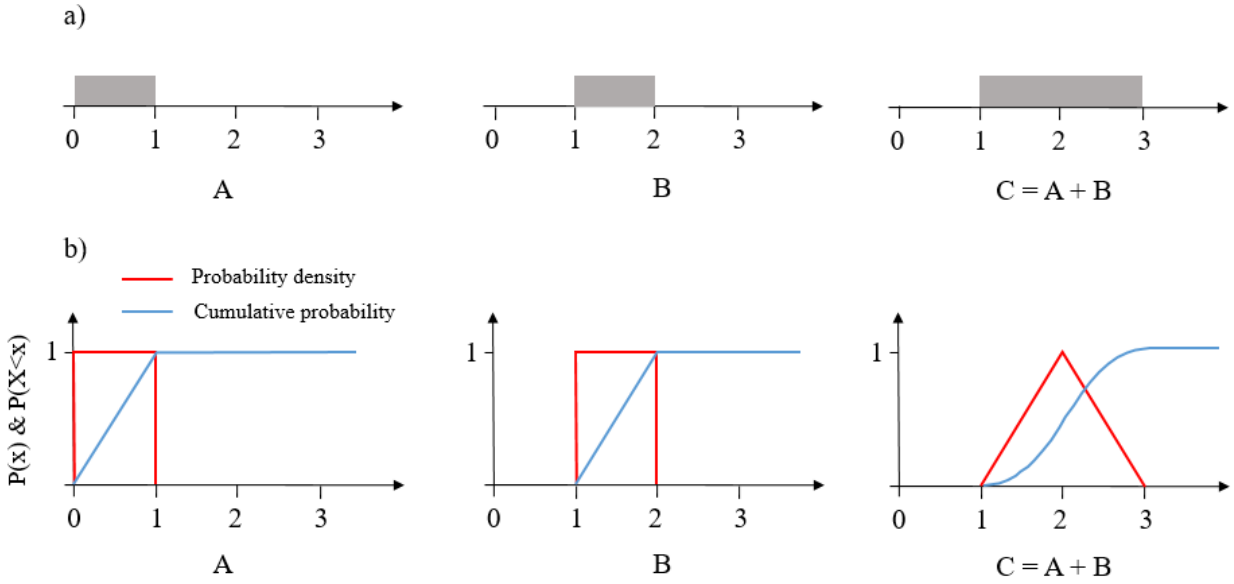

Figure 3 - Illustration of the difference between an interval calculation (a) and the sum of two uniform probability distributions (b)

Note: Probability density represents the probability of the variable taking a certain value, while the cumulative probability represents the probability of the variable being less than a certain value x.

A more "objective" and consistent probabilistic calculation in relation to the information available on A and B would take into account all possible distributions on the supports defined by the intervals, as illustrated in **Figure 4**. This calculation arrives at the same result as the interval calculation of **Figure 3**a.

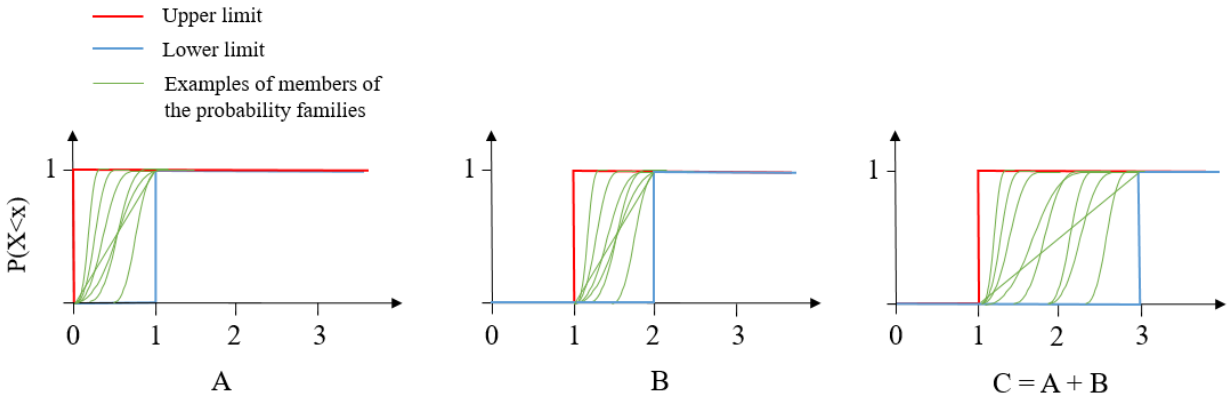

Figure 4 - Calculation based on probability distribution families defined by available information

The non-conservative nature of the subjectivist approach also appears when several subjective probability distributions are propagated, for example using the well-known "Monte Carlo" method (see section 2.4.4), under the assumption of independence between parameters. Due to the multiplicity of probabilities:

P(A and B) = P(A) x P(B), scenarios combining very low-probability parameter values, have very little chance of being drawn in the random sampling process. Yet it is these "outlier" scenarios that are generally the most significant in terms of risk.

These simple illustrations highlight an important question regarding the uncertainty with respect to the value of a parameter X:

- am I not sure of the value of X because it's value is influenced by chance (random variable), but I know its probability distribution?
- or is it because I lack information about X and/or my information is inaccurate?

This question lies at the heart of some of the developments over the past 30 years in terms of representing and propagating uncertainties in model calculations such as risk assessments, with applications in the area of contaminated land.

1.4.2. Recent approaches to the representation and propagation of uncertainties

In the 1990s, Scott Ferson (Ferson, 1996; Ferson and Ginzburg, 1996) who worked in the field of radioactive risks, highlighted the need to distinguish between random variability and ignorance in risk assessments. We also speak of sources of stochastic (related to random variability) versus epistemic (related to partial ignorance) uncertainty. While analysts were well equipped to address random variability, applying classical probability theory, various information theories have emerged since the 1960s to address incomplete and/or imprecise information: possibility theory (Zadeh, 1978; Dudois and Prade, 1988), belief functions (Shafer, 1976), etc., which have strong links and are usually special cases of the more general theory known as "imprecise probabilities" (Walley, 1991). Some of these approaches will be illustrated in the next chapter.

In the field of contaminated land risk assessments, researchers in the early 2000s examined how to propagate both stochastic and epistemic information in risk assessment models. The so-called "hybrid" (Guyonnet et al., 2003; Baudrit et al., 2005) and IRS (Independent Random Sets; Baudrit et al., 2006) methods were developed, with support from ADEME as part of Cédric Baudrit's thesis (Baudrit, 2005) and with applications in the areas of health exposure to soil pollutants or groundwater pollution (Baudrit et al., 2007). These methods have been programmed in the form of an open-access "R" tool, the development of which was also supported by ADEME (Guyonnet et al., 2015; Rohmer et al., 2017).

Further to these developments, hybrid methods have been applied to a variety of fields. Taking into account only the most recent publications, we can cite applications to health risks (Chutia and Datta, 2017), life cycle analysis (Igos et al., 2018), evaluation of ecosystem services (Baustert et al., 2018), atmospheric

dispersion (Abdo et al., 2017) or natural hazards (Tacnet et al., 2017, Dupouy et al., 2017, Tacnet et al. , 2014). But also to domains quite remote from environmental issues, such as the operation of satellites (Toscani et al., 2018), the efficiency of rail transport (Wanke et al., 2018), construction (Islam et al., 2017), the reliability of electrical systems (Jiashen, 2018) or financial risk (Rebiasz et al., 2017).

In areas closer to the management of contaminated land, where geostatistical analysis plays an important role, some research has attempted to take into account the incompleteness of knowledge regarding the variogram (Loquin and Dubois, 2012). Others combined the possibilitistic and Bayesian approaches (Tang et al., 2017) to estimate the ecological risk associated with the presence of certain metals (Cu, Cd and Hg) in soils.

It is understood from the above that there is no single method for dealing with the notion of uncertainty. It depends on the question asked and the information available for addressing that question. The following addresses the issue of uncertainty by starting from the information that is actually collected in a context of contaminated land management.

- The study of the history of science shows that from the beginning of the development of probability theory, this notion is dual: either one models observed frequencies or one evaluates the degree of belief of an individual in the occurrence of an event.
- If uncertainty can be defined as *not being certain*, what is most important in managing uncertainties is the *sources of uncertainty* (the available information). This report considers uncertainties along the data cycle in contaminated land management.
- Different sources of uncertainty warrant different ways of representing uncertainty:
    - If a random phenomenon is described by a sufficient number of precise values (uncertainty of stochastic origin), then classical probability or statistical methods (or geostatistical methods in the case of spatial variability) should apply.
    - If, on the contrary, we are dealing with sparse or imprecise data, or expert judgment (uncertainty of epistemic origin, because related to the incomplete/imprecise nature of the information available), then other tools may be better suited for representing uncertainty (possibility theory, belief functions, imprecise probabilities, ...).
- In the area of contaminated land management, consistent approaches to uncertainty are needed for a reliable reporting of data and results of predictive modelling and risk assessments, in order to promote management decisions that are robust and in line with available information.

2. Uncertainties along the data cycle in contaminated land management

2.1. Introduction

For the purpose of readability, the data cycle in a context of contaminated land management in **Figure 1** is presented below with the section numbers corresponding to the different stages of the cycle.

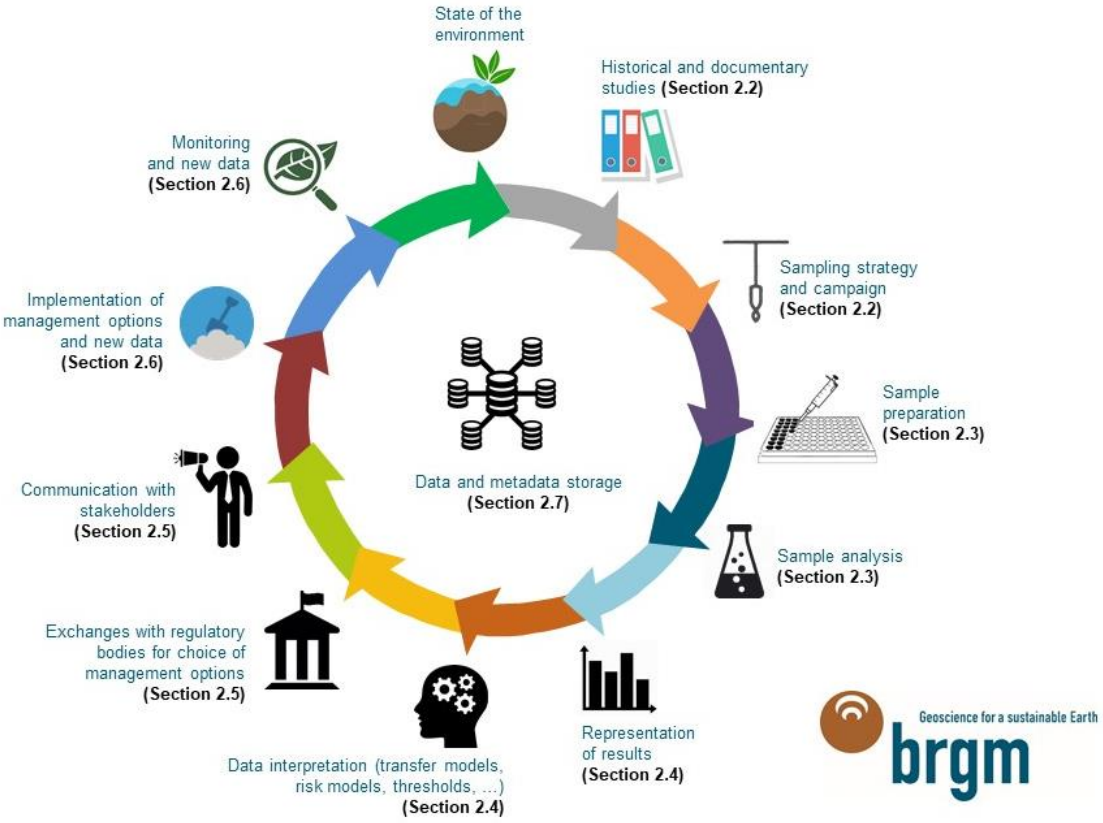

Figure 5 - Environmental data cycle in the context of managing contaminated land

While this chapter covers the uncertainties involved and methods for addressing them, Chapter 3 summarizes proposals for further research identified for the various stages.

2.2. Documentary studies and sampling

2.2.1. Historical and documentary studies

In the practice of managing contaminated land, historical and documentary studies are used in particular at an early stage in order to guide the investigations. They consist mainly of identifying activities carried out on a site, the locations of the various facilities (e.g., for chemical storage), the evolution of their spatial spread over time, past incidents or accidents, the use of backfill materials and which pollutants might be encountered both on-site and in the surrounding areas, etc. If these studies are not properly carried out, e.g., by neglecting certain historical activities on the site or the types of chemicals stored, etc., the resulting uncertainties may have very important consequences on subsequent land management decisions.

Historical and documentary studies therefore have a major influence on the uncertainties that affect a project. They are used, at a very early stage of a project, to determine whether the site is potentially contaminated or if contamination is proven. Indeed, the first action described in standard NF X 31-620-2 (AFNOR, 2018) is "elimination of doubt", which illustrates the importance given to uncertainties in the recommended approach, starting from the early stages of a study.

2.2.2. Soil sampling

a) Context and sources of uncertainty

While environmental chemical analysis laboratories have long been accustomed to estimating their measurement uncertainties (see section 2.3), the situation is quite different for other players in the area of contaminated land (consulting companies, remediation companies, etc.). This does not result from a lack of motivation on the part of these actors, but rather from the overall complexity of a contaminated site (subsurface heterogeneity, spatial extent of contamination, constraints regarding access to the contaminated area, etc.) and also from a lack of tools and measurement frameworks for a reliable quantification of uncertainties during the sampling phase.

However, the profession applies tacit rules for qualitatively assessing the influences of certain practices. With no claim to completeness, the main sources of uncertainty that could affect sampling and therefore, more generally, influence contaminated land management, can be listed as follows:

- during the historical and documentary study, where the identification of activities, substances (see http://ssp-infoterre.brgm.fr/matrice-activites-polluants) and practices that are likely to generate contamination, depends on the information collected, their quality and the possibility of cross-comparison;
- when describing the environmental context, for which intrinsic heterogeneity is an important source of uncertainty and which is often not known at the appropriate scale (for example, the direction of groundwater flow in the heart of a city versus regional flow or the delineation of an off-site contaminant plume);
- during the investigation phase, i.e. during the acquisition of data from the subsurface of a site, uncertainties arise due to various aspects such as the difficulty to access specific areas of the site, the collection of samples at a moment in time, when in fact the system is dynamic (groundwater, soil gas, indoor air, …), the representativeness of investigations carried out according to the sampling strategy and often in a constrained timeframe (sampling depths, number of samples, size of the samples, ...) or the sampling techniques used (sampling protocols, conditioning, packaging, transport);
- the delays between the investigations and the actual site remediation works also generate uncertainty since this discrepancy, which may be on the order of several months or years, does not take into account how the contamination has evolved in the interval. The site will thus be characterized at some point in time and management scenarios will be established, but their effective implementation might be carried out under very different conditions and with a much greater extension of contamination than the one initially anticipated;
- during remediation works, where it is common to define safety margins based on assumptions regarding the design of the remediation site or processing units, in order to have some latitude in the event that certain factors of influence derived from laboratory and/or field tests are not fully satisfied (treatment well ranges of influence, extraction rates, biodegradation kinetics, etc.);
- finally, during the reception of works, the uncertainties associated with sampling are also very important as they depend on the number of checks performed, on the protocols used, and also on the variability of concentrations for a given context (it may also be necessary to take into account rebound effects).

b) Managing uncertainties during the soil sampling phase

Obligations associated with soil sampling?

There is currently no methodological guidance document for managing uncertainties over the entire course of a project related to contaminated land sampling, or to contaminated land management in general. The identification of uncertainties and their influence on results are nevertheless considered in the French national methodology for managing contaminated land (April 2017) and also in several items of standard NF X 31-620 (comprehensive and elementary services in sections 2 and 3 of this standard: A200 and following; A270, B120 and B130, ...).

It is required in particular that following sampling, measurement, observation and/or analysis of contaminated media, consultants discuss the uncertainties affecting the results, considering in particular the methods or equipments used. Also, during the interpretation phase of the results (service A270 of the standard), a presentation of the limitations and uncertainties arising from the investigations carried out and a discussion of their influence on the results, are requested.

At an international level, the notion of uncertainty during the sampling phase is addressed in at least two standards: NF ISO 18400-102 (§ 5.3; ISO, 2017a) which addresses the choice and implementation of sampling techniques and NF ISO 18400-104 (§ 5.8; ISO, 2017b) which deals, in particular, with possible sampling strategies. The latter document also presents an annex (informative) dedicated to the evaluation of the sampling uncertainty and proposes different methods for improving characterization (duplicate sampling methods, OCLI method, ...).

Finally, it is worth mentioning some specific standards for certain sampling practices, such as ISO 22155 (ISO, 2016): "Soil quality - Dosage of volatile aromatic and halogen hydrocarbons and certain ethers by gas phase chromatography - Static headspace method," which defines requirements in terms of soil sampling methods for the investigation of volatile compounds, to limit losses (in particular by volatilisation) and therefore to reduce uncertainties during the sampling phase.

Inter-comparison of soil sampling techniques

At the French level, two studies focused more specifically on comparing soil sampling protocols for the analysis of organic compounds (particularly volatile compounds). These include:

- A study performed by Burgeap for ADEME (ADEME-BURGEAP, 2015);
- A study performed by BRGM for the French Ministry of Environment; MTES (Favereaux et al., 2019).

Figure 6 shows the area investigated during the BRGM inter-comparison trial in 2018. These studies applied, in the field and for several soil contexts, distinct coring (continuous-flight auger, core liner, windowless sampling core) and sampling methods (jars, sampling cylinders, jars pre-filled with methanol). Illustrations of the coring and sampling methods used in the trial are presented in

Windowless sampling core Core liner Continuous-flight auger

Figure 7 and **Figure 8**.

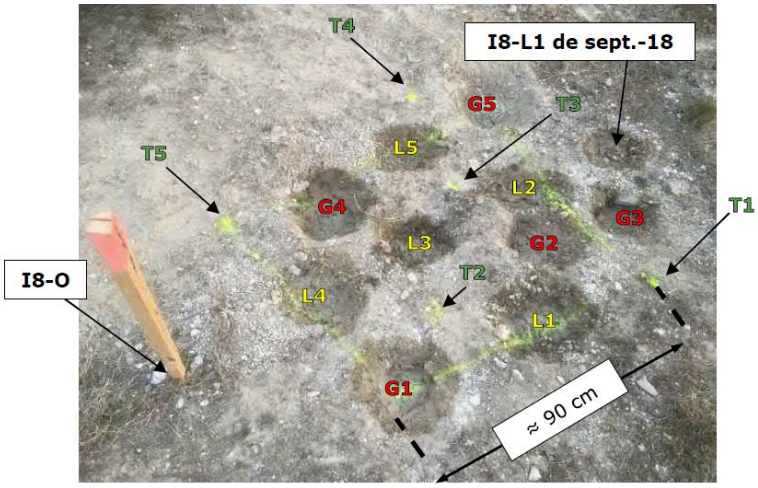

Figure 6 – View of an area investigated during the BRGM inter-comparison test (2018)

Windowless sampling core | Core liner | Continuous-flight auger

Figure 7 – Different investigation methods used for the BRGM inter-comparison test (2018)

Results of these studies do not allow an accurate quantification of the uncertainties associated with sampling methods and sampling practices: there is currently no template or method for equating a specific sampling technique or method to a precisely quantified uncertainty. Nevertheless, despite occasionally different results depending on the context (e.g., the type of matrix; sands, silt, marls, …), these studies lead to recommending the use of multilevel lined core sampling for characterizing and delineating sources of volatile compounds. It helps to better preserve the integrity of soil samples by avoiding the loss of structure and hence of volatile compounds.

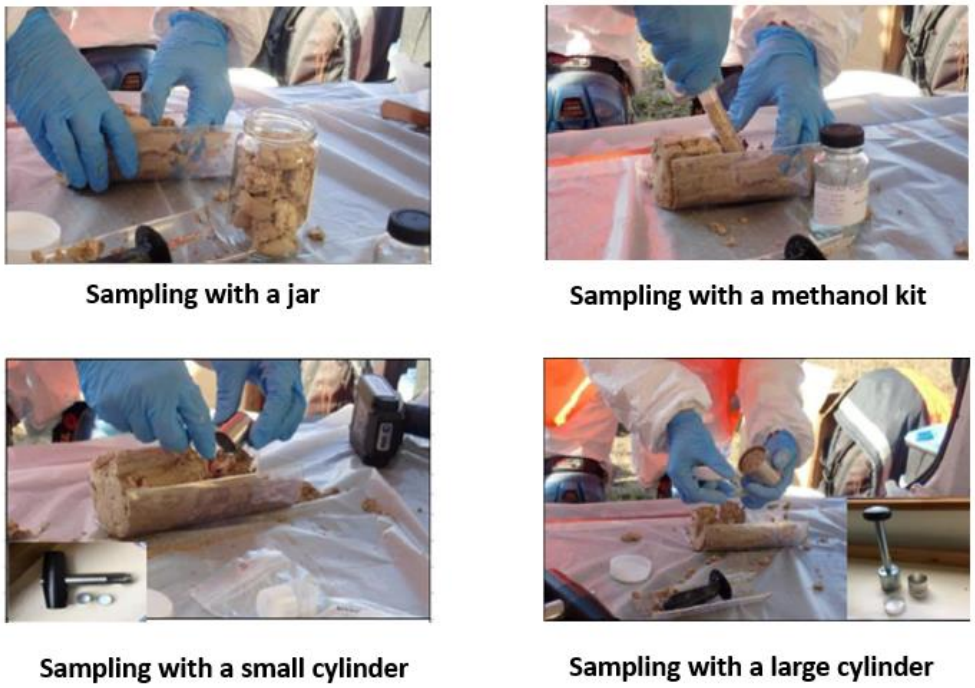

Figure 8 – Sampling methods used in the BRGM inter-comparison trial (2018)

With respect to soil sampling, the studies illustrate the relevance of the methanol kit method (jar pre-filled with methanol) for a finer characterization of volatile compounds (and to quantify concentration variability), and of the 16 ml stainless steel cylinder for certain soil types. The use of a simple jar, which remains a widely used method, seems more restricted to identifying the presence of pollutants rather than accurately characterizing their concentrations. This method requires a rigorous protocol to minimize losses through an alteration of soil structure and exposure to air. It should be used preferably for less volatile compounds (Total Hydrocarbons C10-C40).

The tests also showed that the point of sampling within a soil core is paramount and requires a lot of experience on behalf of the operator. It is recommended in particular to repeat soil samples to improve representativeness. Indeed, significant variations were observed within a core of 1 m length which was initially assumed to be homogeneous in terms of concentration and lithology. These variations are related to soil heterogeneity and differences in pollutant behaviour/mobility and should be taken into account in the sampling strategy.

A cross-comparison between the various results of these studies (ADEME and BRGM) and those of other trials that might be available, remains to be carried out in order to develop a guide of good practice taking into account the variety of situations in the field (nature of the contaminants, lithologies, ranges of concentrations, ...). Such work is expected to be performed in the course of 2020 and early 2021.

Some recommendations to limit the uncertainties associated with soil sampling

While global uncertainties combine elements of uncertainty arising both from the analytical uncertainties associated with laboratory operating procedures (including the sample preparation phase; see section 2.3) and uncertainties related to the phase of sampling in the field, it is recognized (see NF STANDARD IN ISO 18400-104) that the latter are generally the most significant and difficult to estimate. In order to minimize these uncertainties, a number of recommendations can be proposed[1]:

[1] Recommendations are not in increasing or decreasing order of associated uncertainty.

1. densify the number of sampling points in a given area. Various guidance documents recommend the collection of sample clusters, to avoid that a management strategy should rely on just one or a few samples;
2. ensure continuity between field operators. Indeed, increasing the number of operators in the field can lead to differences in sampling protocols and hence to a larger variability of results (e.g., sampling targeted specifically on the contamination versus on a certain type of soil, single sample versus composite sample, ...);
3. in connection with the second point, prior to on-site investigations define a sampling protocol that is suited to the context and type of pollutants involved, then retain this same sampling protocol throughout and, when possible, the same analytical laboratory (and hence the same methods for sample preparation and analysis);
4. take into account the grain size of soil particles in the samples that the laboratory will prepare and analyse. While it is generally recognized that contamination is concentrated in the fine fractions (less than 2 mm), the practice of sifting soils before sampling for analysis is not always appropriate as it may have a strong influence on mass balances and the extrapolation of concentrations measured on the fine fraction to the entire mass sample and, further, to the estimation of volumes of contaminated soil to be managed (cf. ADEME's ongoing CAFRAGES project). Conversely, this same fraction lower than 2 mm might be considered too coarse in the case of exposure to soil by ingestion of soil particles for which, according to the relevant literature, the focus should be on the fraction less than 250 μm (or finer);
5. to have an integrated view of the environmental situation, through the use of an adequate conceptual model: this requires in particular correlating concentration data obtained in soils and water with data available for other media (e.g., soil gas in the case of volatile organics, or even indoor air), to help better understand the contaminant migration mechanisms involved and to improve the relevance of health risk estimations;
6. to combine field measurements and the collection of samples for analysis in the laboratory. This approach leads to an optimization of the investigation program by increasing the number of field measurements and improving their reliability through verification with laboratory analyses. It is important to establish the correlation between different analysis methods and to perform adequate calibration of field measurement devices taking into account the specific context (as in the case of, e.g., portable X-ray fluorescence spectrometers);
7. to carry out sequential operations with as little time as possible between them, in order to limit the influence of evolving environmental conditions. This is particularly sensitive in the case of dynamic environments such as surface water or soil gas;
8. gather temporal data, to allow conclusions based on data chronicles and the identification of trends, rather than to conclude based on just a single set of data obtained from a single measurement campaign. While this statement may seem obvious, it is clear that the constraints affecting contaminated land investigation projects; e.g., tight schedules for on-site sampling campaigns, must be taken into consideration. It is nevertheless worth reminding considering its importance for various contexts (e.g., health risk assessments, receipt of remediation works, ...). However, depending on the uncertainties that persist further to the assessment of remediation works, the implementation of a program for monitoring the quality of certain environmental media can help consolidate the results and improve the management of the contamination.

2.2.3. Groundwater sampling

Groundwater sampling is very specific for at least two primary reasons: (i) the distribution of groundwater concentrations is influenced by groundwater flow directions and (ii) the thickness of the aquifer may be significant. Regarding the first point, uncertainty is mainly generated by the multiscale variability of hydraulic conductivity (Bayer et al., 2011) which is typically related to the notion of large-scale dispersion (Gelhar et al., 1992). While there is an abundance of theoretical studies on this issue, they are often difficult to transpose from one site to another (Dagan, 1990). Thus, with respect to sampling, the theoretical "spatial continuity" of a contaminant plume does not help to precisely position drill holes and there can be

concentration differences of one or more orders of magnitude over distances of only a few metres. In some cases, there is also a temporal variability of concentrations in relation with changes in flow directions (Goode and Konikow, 1990).

Even more significantly, most studies show vertical concentration variability that can reach several orders of magnitude, especially in areas close to the contaminant sources. This variability stems both from the heterogeneity of the subsurface but also, in the case of organic pollutants, from the mechanisms of organic pollutant infiltration into the subsurface as a pure phase (Côme et al., 2006). In the presence of vertical variability, the selected sampling technique will of course have an impact on the measured concentrations. This is why multi-level piezometers are commonly used for research purposes and also in practice on many North American sites (Puls and Paul, 1997).

Some reports and publications provide information regarding the orders of magnitude of the variability to be expected. Close to the contaminant source areas, concentrations may vary by a factor of 100 over a soil thickness of only 1 to 2 m (Rivett et al., 2001). Due to low vertical- and horizontal-transverse dispersion, the interface between a contaminant plume and uncontaminated groundwater is often only a few centimetres thick in the vertical direction (Klenk and Grathwohl, 2002) and a few decimetres thick laterally (Harvey and Gorelick, 2000).

Comparisons have been made between different sampling methods and their influence on the uncertainty relative to measured groundwater concentrations (Barnier et al., 2013; Dubearnes et al., 2005; INERIS, 2018; Kulkarni et al., 2015; Quiot and Guerin, 2018; Rollin et al., 2008). There currently does not, however, appear to be a synthesis of these various studies that might help derive consolidated data regarding uncertainties.

2.2.4. Sampling of soil gas and indoor air

Sampling soil gas or indoor air inside a building generates specific problems in terms of uncertainties, related in particular to the strong variability of both spatial and temporal pollutant concentrations in this context. Spatial variability is primarily the result of the spread of contamination, the multiscale variability of subsurface properties (heterogeneity) but also of the spatial distribution of organic contaminants. In terms of variability orders of magnitude, the relevant literature shows that soil gas concentrations may vary by a factor of 100 over just a few meters of soil thickness (see for example **Figure 9**).

The temporal variability of gas concentrations is influenced by the various mechanisms acting on the system at hand, which includes *a minima* the soil, the water table and soil air but also, in the case of a building, the basal concrete slab and the indoor air. For concentrations in soil gas or indoor air, 4 time scales should be considered:

- hourly (immediate effects associated with a change in pressure or with ventilation);
- daily (diurnal cycle associated with day/night variations in weather conditions);
- multiday (related to, e.g., an equilibration of pressures following rainfall, etc.);
- seasonal (related to, e.g., variations in diffusive or advective vapour transport).

Conceptually, the transport of soil gas is induced by the following hydro-meteorological phenomena: rain infiltration, water table variations, changes in atmospheric pressure and wind speed. And the factors to consider in priority are: temperature, soil water content, groundwater table level, atmospheric pressure and wind speed.

With regard to indoor air, the factors to be considered as a priority are on the one hand those described for soil gases and on the other hand those related to the building; its ventilation, heating (variability of the thermal budget), etc. but also factors associated with occupant behaviour (smoking, use of room diffusers, storage or use of cleaning products, etc.). The graphs below illustrate temporal variations in concentrations measured in soil gas and indoor air that exceed a factor of 10 at time scales of a few months in the case of soil gas and of only a few hours for indoor air.

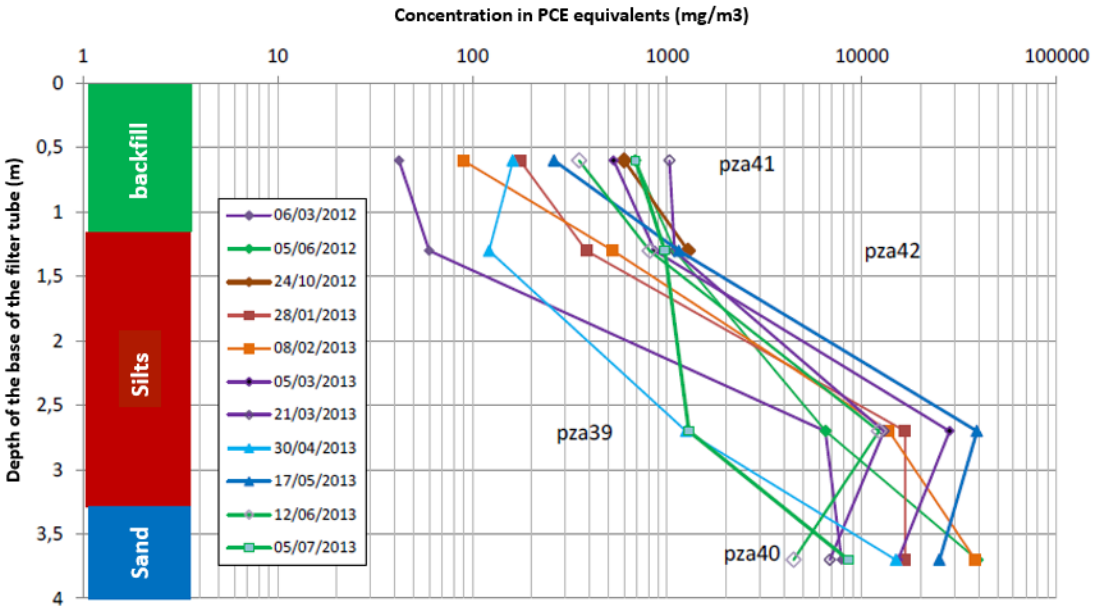

Figure 9 – Spatial and temporal variability of soil gas concentrations measured using a photoionization detector (PID) in a quadruplet of air piezometers (FLUXOBAT test site; Traverse et al., 2013)

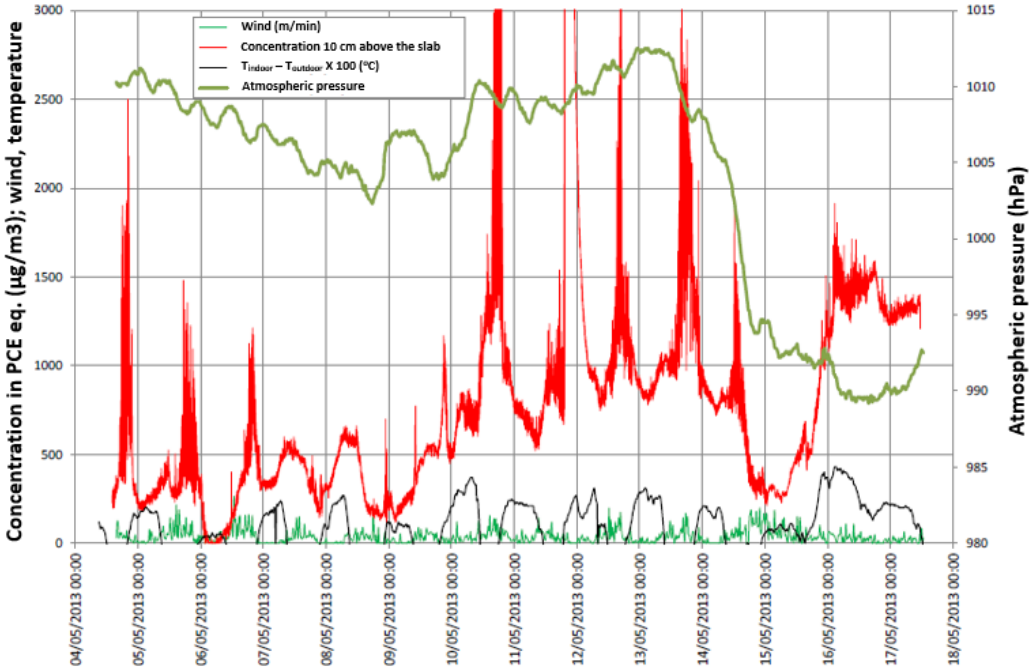

Figure 10 – Influence of wind and pressure on indoor air concentrations (FLUXOBAT test site; Traverse et al., 2013)

- In the absence of a generally accepted methodological guide, but also considering the large number of factors of influence, the uncertainties associated with the contaminated soil sampling phase are rarely addressed in a quantitative fashion as part of current practice in contaminated land management.
- Sources of uncertainty that can affect sampling range from the quality of historical and documentary studies, to the consideration of the heterogeneity and dynamics of the studied environmental media (contamination in soil, groundwater, soil gas, etc.) and the applied sampling and conditioning methods, etc.
- With regard to the sampling of soils contaminated by volatile organic compounds (VOC, BTEX), inter-comparison tests can help highlight the advantages of certain methods such as the use of jars pre-filled with methanol.
- Additional good practices can help reduce the uncertainties associated with the contaminated soil sampling phase, such as the association of field measurements (which can be in greater numbers) and laboratory measurements for a validation of field measurements, taking into account the grain size of the analysed fractions to avoid assigning certain test results to irrelevant soil volumes, or an adequate sequence of field operations to avoid delays during which the situation in the field might evolve.
- In groundwater there are often strong spatial variations in concentrations, especially in areas close to the pollutant sources, where concentrations may vary by a factor of 100 over thicknesses of only 1 to 2 m.
- In the case of concentrations in soil gas or indoor air, spatial variations can be accompanied by strong temporal variations, particularly in relation to hydro-meteorological phenomena.

2.3. Sample preparation and analysis in the laboratory

2.3.1. Introduction

The uncertainty determined by the analytical laboratory usually only addresses the final analytical step applied to the so-called "sample-for-analysis" (or in some cases sub-sample) and does not necessarily take into account the physical preparation step. On the other hand, it does account for the entire analytical protocol, i.e., extraction (if any) and the final instrumental analysis.

Physical preparation step

The following physical preparation steps are currently rarely considered when assessing laboratory-uncertainty:

- **Subsampling**: a portion of the initial sample received by the laboratory is subsampled to provide the quantity required for the analysis, according to the laboratory's protocol. For example, for water samples, the volume processed is generally smaller than the volume requested by the laboratory, to allow for duplicate analyses in the event of difficulties. For soils, the laboratory will usually prepare or analyse only a portion of the mass received, in order to preserve original material, or to optimize preparation time. The standards for analysis or preparation of solid materials specify how to obtain a representative subsample. The initial sample may thus be divided into several subsamples (e.g., a subsample for the analysis of volatile compounds, another for PAH analysis, another for TOC, etc.).

- **Physical preparation:** this step depends on the parameters to be analysed and on the matrix. It can be carried out on the entire sample received, or on a subsample. Soils can undergo steps of, e.g., drying, quartering, homogenization, grinding, while water samples can go through a filtering step. The sample prepared for analysis is therefore physically different from the initial sample (in terms of granular size, water content, suspended matter content, etc.).

Analysis step

As stated above, the measurement uncertainty determined by the laboratory mainly refers to the analytical protocol applied to the prepared sample (namely extraction, if any, and analysis). Environmental chemical analysis laboratories have long been used to estimating their measurement uncertainties. However, the requirements of quality assurance systems (agreement) and regulatory rules, have increased significantly since the years 2000. Uncertainties are essential information to associate with an analytical result, in order to appreciate the level of confidence in a result and to be able to use it correctly (in addition to information on the method used, limits of quantification, etc.).

Uncertainty estimates:

- enable analysis results to be compared with threshold values (regulatory or not), in terms, e.g., of the risk of exceeding such values. In this case, standard and/or regulatory documents should describe how uncertainty must be accounted for in the comparison;
- are essential information for designing trend monitoring programs: they affect the ability to detect future trends (upward or downward), choices relative to data acquisition frequencies, monitoring duration, the intensity of expected variations (the larger the uncertainty, the smaller the chances of identifying trends and therefore the more data will be needed and over longer periods of observation);
- allow the comparison between results, to assess whether observed differences are significant (for, e.g., controlling results from two different laboratories that have analysed the same sample, or for comparing analyses performed at two different moments in time). Without information on uncertainties, such comparisons are impossible.

2.3.2. Main sources of uncertainty

In a context of laboratory analyses, a significant number of sources may contribute to the overall uncertainty. Examples include:

General

- Inaccuracy in the definition of "the quantity to be analysed" (the measurand[2]).

Physical preparation step:

- poor representativeness of the sample taken for analysis, with respect to the sample actually received (due, e.g., to inadequate quartering, grinding, etc.);
- losses of contaminant occurring between the sampling and final analysis steps (due to, e.g., degradation, volatilization, precipitation, etc.);
- risks of sample contamination (by the operator, the atmosphere, from reagents, etc.). Such risks are more important for certain families of parameters (plasticizing compounds such as phthalates, PAHs, VOCs, certain metals, etc.) and in situations where concentrations are low. Cross-contamination between samples of very different concentrations may also occur. And it is worth mentioning the special case of vegetable preparation for analysis (washing, peeling), as only a small amount of residual soil may strongly impact analysis results.

[2] The measurand is the quantity intended to be measured. It may differ from the quantity that can actually be measured

Chemical analysis step:

- biases related to the extraction stages (e.g., bad estimation of extraction yields, complexity of the estimation in the absence of reference materials);
- calibration errors (purity of standards, ...);
- errors in instrument metrology (temperature, volume, mass, etc.) ;
- methodological errors (e.g. dilutions).

In general, sources of uncertainty can be grouped into 5 classes: Environment, Method, Object, Operator and Instrument.

2.3.3. Uncertainty management

As noted in paragraph 2.3, laboratory uncertainty assessments focus mainly on the "final analytical" protocol and rarely on the physical preparation phases.

a) Obligations for laboratories

Almost all environmental analysis laboratories work under an agreement framework (COFRAC in France). Laboratories must demonstrate compliance with the requirements of standard NF EN IEC 17025, which requires laboratories to estimate their uncertainties and to identify contributions to these uncertainties. It also requires that these uncertainties be included in the test report if:

- it is important for the validity or the applicability of test results;
- it is a request of the client;
- if measurement uncertainty affects compliance with a specific standard.

In addition to this overall quality assurance framework, several regulatory texts in the context of environmental or health protection have reinforced the requirements for laboratories regarding measurement uncertainties. The European Water Framework Directive (2000/60/EC) has emphasized the importance of measurement quality, their reliability and their comparability (see Ghestem, 2011). It has thus led to the development of a specific directive on quality assurance and control (2009/90/EC). Laboratories operating under these guidelines must guarantee uncertainties below specific values relative to the EQS standards (Environmental Quality Standards for surface water) or to groundwater quality standards. At the French level, the ministry for the environment's agreement procedure has adopted this requirement and made it one of the conditions for laboratory agreement. This only applies, however, to substances and matrices (water, sediment, biota) covered by this agreement.

b) Concept of uncertainty

Any measurement process is subject to factors of influence referred to as "sources". These factors of influence are more or less well controlled (or controllable) by the operator. Thus the measurement result is not a unique value. Variations between repeated measurements occur because the factors affecting measurement results are not maintained perfectly constant. This introduces "doubt" with respect to the final result. The purpose of the uncertainty estimation is to characterize this doubt.

Schematically, a measurement result can be broken down into three components (**Figure 11**):

- the measurand's "true" value, which is most often unknown or very difficult to access;
- a component related to systematic errors that is the same with each new measurement;
- a component related to random errors that fluctuates unpredictably with each new measurement.

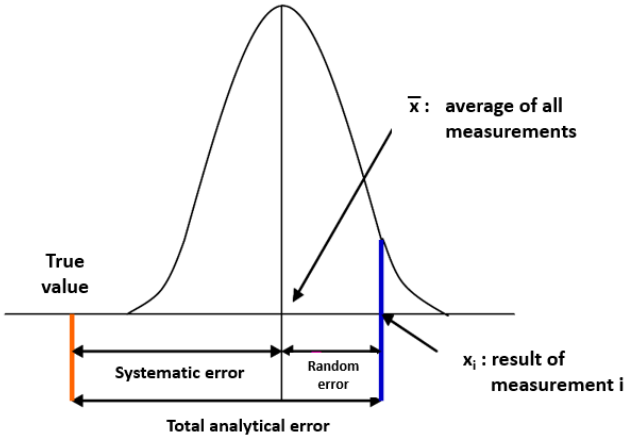

Figure 11 - Schematic representation of laboratory uncertainty (modified from Ghestem and Lachenal, 2008).

The results are more or less dispersed (concept of precision) around an average value that is itself more or less remote from the "true" value (concept of trueness or bias). The diagrams below, based on the image of a target centred on the "true" value, illustrate these concepts.

Figure 12 – Different types of uncertainty associated with laboratory measurements (modified from Ghestem and Lachenal, 2008).

A correct estimate of uncertainty should take into account both systematic and random sources of error. Uncertainty depends on:

- concentration levels: it is larger at concentrations close to the limit of quantification (LOQ) than at higher concentrations;
- the method used: for example, uncertainty is often larger in the case of manual methods compared to automated methods, but it can also be very different in the case of two automated methods based on different principles;
- the laboratory: uncertainty depends on the laboratory's efforts to improve its analytical methods (control analyses, duplicates, use of certified reference materials, staff qualification,...);
- the matrix: for equivalent analyses conditions (parameter analysed, concentration level, method, etc.), results will not be the same following the nature of the matrix involved: drinking water versus waste water or brines in the case of a liquid matrix, or sand versus clay in the case of a solid matrix. In practice, laboratories assess uncertainties for groups of samples of similar characteristics;
- how the uncertainty is estimated. In theory this should not be the case, but in practice this aspect might influence the laboratory's ability to perform the uncertainty calculation, or the applied uncertainty estimation method might have an influence (for this reason, uncertainty should not be, with exception, a criterion for the selection of laboratories, or if it is then the criterion should be used with caution).

Analyses results should be provided with the associated uncertainty in order to be able to interpret them correctly. A lack of information regarding the level of concentration at which an uncertainty is estimated, makes the estimation unusable.

A very important point is the way in which uncertainty is expressed and the notion of “uncertainty coverage factor”. From its estimation of uncertainty, the laboratory obtains a "standard uncertainty," noted “u”, which is often derived from a standard deviation. The "final" uncertainty is generally expressed in the form of an expanded uncertainty “U”, which is a multiple “k” of the standard uncertainty “u” (usually, k = 2). With k = 2, the probability that the "true" measured result lies within the range "result ± U" is 95% (assuming a normal distribution). It would be only 68% if “k” were taken as 1. Without information on this coverage factor, the uncertainty provided by the laboratory cannot be interpreted.

Estimating measurement uncertainty is a complex task that often requires the acquisition of a large amount of data. Standard documents provide the principles and methods for estimating these uncertainties. Among the most noteworthy standards in the field of water analysis are: NF EN ISO 11352 (AFNOR, 2013) and EURACHEM / CITAM (LNE, 2012). The methods either consider the uncertainties associated with each source of uncertainty and then combine them into a global uncertainty, or else, more pragmatically, estimate directly the global uncertainty based on estimates of the “precision” and "trueness" of the process. It is this latter approach that is currently widely used in laboratories through the application of the NF EN 11352 standard.

c) Inter-laboratory trials

Each year in France and Europe, an important number of inter-laboratory trials are organised by inter-laboratory comparison agencies (ILCAs); such as AGLAE and BIPEA in France. These events help laboratories check the reliability of their results on a regular basis, through external testing. The results obtained by the laboratories during the trials are used as criteria for their agreement by the French ministries of environment and health.

In addition to their objective of assessing the laboratory's ability to provide reliable results, these inter-laboratory tests provide extremely valuable information regarding the dispersion of laboratory results. This dispersion is sometimes referred to as the "profession’s uncertainty": it provides managers or decision-makers with an estimate of the profession’s ability to provide reliable results for a given parameter in a given matrix.

In the field of water analyses, AQUAREF, in collaboration with ANSES and AGLAE, summarized the observed dispersions for more than 150 parameters (Moreau et al., 2019). For each parameter, the dispersion of results observed in the AGLAE inter-laboratory trials are provided at concentration levels that correspond to regulatory threshold values for environmental media. The considered media are: surface water, groundwater and water for human consumption. Dispersions are provided with a coverage factor of 2 (which corresponds schematically to a 95% confidence level). Taking as an example lead concentrations in groundwater (for which the regulatory threshold is 10 g/L), 95% of laboratories obtained an analysis result located within the interval 10 ± 1.8 g/L.

This type of information could be made available to managers and decision-makers to inform them regarding the level of reliability of analytical results. Additional syntheses could be carried out for other parameters of interest in a context of contaminated land management, or for other matrices (soils, sediments, air, vegetable plants), provided inter-laboratory test data are available.

- In the field of analysis, there are multiple sources of uncertainty related in particular to the sample preparation steps: poor representativeness of the subsample taken for analysis, losses between sampling and analysis (degradation, volatilization, etc.) and to the analysis itself (contamination by the operator or the atmosphere, calibration errors, etc.).
- The uncertainties currently estimated by laboratories take only (or primarily) into account the final “analytical" steps that follow the sample preparation. The physical preparation of the sample prior to analysis is not usually taken into account.
- The measurement uncertainties determined by the laboratory are essential information that should accompany the actual analysis result, to be able to account for the possible dispersion of the result.
- It is important to specify how uncertainty is expressed and in particular which coverage factor was used (usually a value of 2 according to current standards).
- Uncertainties vary depending on the parameter concentration level, the method of analysis or the matrix analysed (water, soil, …).
- Inter-laboratory testing is an essential tool for improving the quality of data because it provides an estimation of the “profession’s uncertainty”. It is essential that such comparison trials be maintained, or developed when they do not yet exist for certain parameters.

2.4. Data representation and interpretation

2.4.1. Precise, random and imprecise parameters, …

Precise parameter:

A parameter may be precise: for example, the speed of light is equal to 299792458 m/s. Regardless of location or measurement reference and notwithstanding experimental errors, measuring the speed of light will yield this or an approaching value. The degree of accuracy required (e.g., the number of significant digits) depends on the application area (calculating the distance of a star, GPS applications, etc.).

Random parameter:

But few parameters in nature have such precisely-known values. Taking for example the 10-day rainfall depth in Orleans over the period 1992-2018, measured values yield the frequency histogram in **Figure 13a**, which suggests that the random variable "10-day rainfall depth" follows a log-normal type of distribution. **Figure 13b** shows the same data in the form of a cumulative relative frequency distribution. Equating this distribution with a probability distribution, the graph suggests that if we randomly select a 10-day period between 1992 and 2018, we have a 50% chance that the rainfall depth is less than 13.2 mm and a 95% chance that it is less than 50.6 mm.

To use this type of information in a risk model in a context of contaminated land management, one can either use the measured values directly, or fit a probability distribution to the measured data. **Figure 14a** shows the result of an automatic fit (using an optimization algorithm) of a log-normal probability distribution to the measured data. It is seen that the fit is not very satisfactory. A superior match is obtained using a Gamma probability distribution (**Figure 14b**), which is defined by two parameters: a parameter of shape (in this case: 0.86) and of scale (in this case: 22.54).

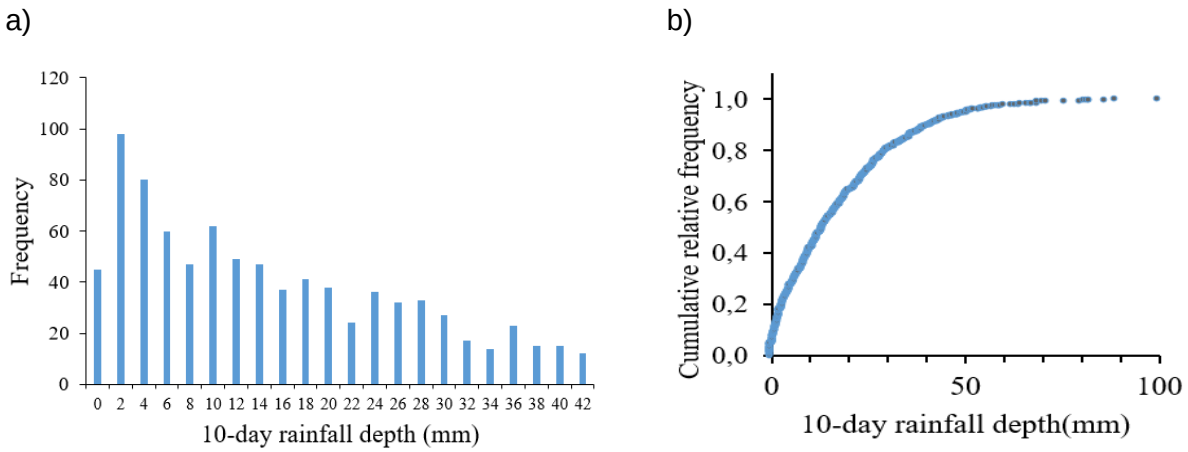

Figure 13 - Histogram of frequencies for 10-day rainfall depth measured in Orléans over period 1992-2018 (a) and distribution of cumulative relative frequencies (b).

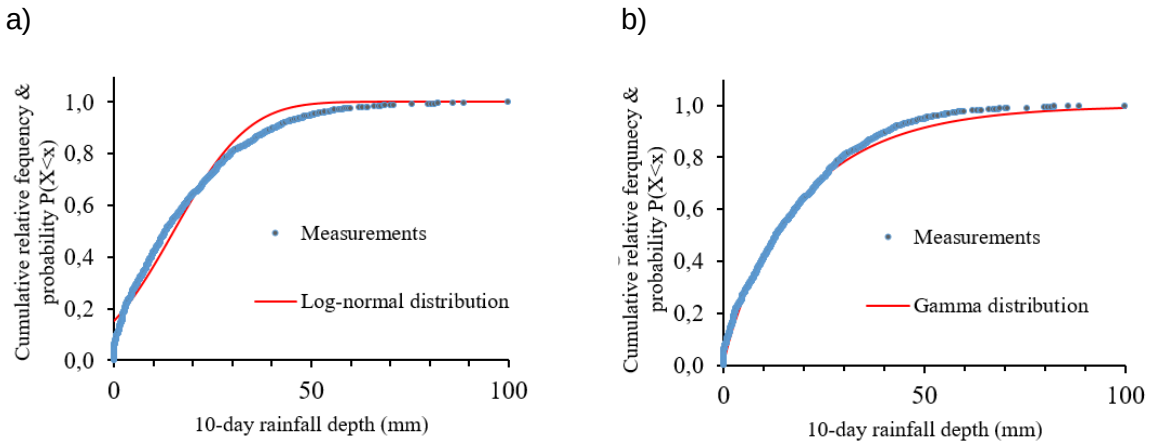

Figure 14 - Automatic calibration of the frequency distribution using a log-normal probability distribution (a) and a Gamma probability distribution (b).

This process of fitting a single probability distribution to measured data is possible, on the one hand, because there is a sufficient amount of data available and, on the other hand, because rainfall depth is a variable that is well defined and easily measured. In other situations, we might be dealing with sparse and incomplete measurements, or else with measurements in sufficient numbers but that are not precise. **Figure 15a** shows the calibration of a normal probability distribution to arsenic concentration data measured on a mine tailings heap. The best calibration, using an objective function minimization algorithm (a sum of squares of differences), is obtained for an average value = 83.5 mg/Kg and a standard deviation = 35.7 mg/Kg. But as measured values show some dispersion around this distribution, one might prefer to fit the data using a "parametric" probability family (Baudrit et al., 2008) as shown in **Figure 15b**, where the measured values are delineated by an upper and a lower probability distribution, obtained by defining intervals of possible values for the average concentration: [68-100] mg/Kg and for the standard deviation: [34-36] mg/Kg. These limiting distributions define a "family" of probability distributions, composed of all the distributions located between the upper and lower bounds, analogous to the notion of imprecise probability (Walley, 1991) or to the "p-boxes" of Ferson and Hajagos (2004).

As shown in the next chapter, such modes of representation can be used for various types of analyses, such as environmental or health risk assessments. They can be used to determine, e.g., cut-off thresholds from mass balances and applying the so-called "Pareto" principle, which proposes that, on average, 80% of the effects are the consequence of 20% of the causes (applied to the management of contaminated land, this principle suggests that 80% of the contaminant load is typically associated with only 20% of the soil volume; Lion et al., 2016).

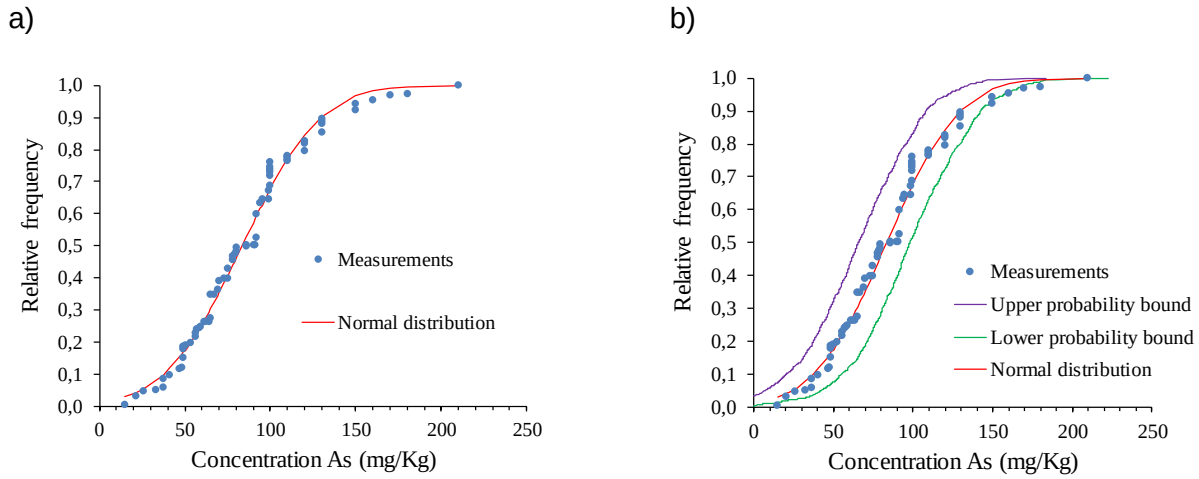

Figure 15 – Fitting of arsenic concentration measurements in a mine tailings heap using a normal probability distribution (a) and bounding of these measurements using a parametric family of normal distributions (b).

Imprecise parameter:

The above discussed precise parameters (example of the speed of light), followed by random variables, represented by conventional (single) probability distributions, and finally families of probability distributions. But in some cases we do not have significant amounts of data, whether accurate or not, but only very partial and/or imprecise information, as is the case with, e.g., expert judgment. In this case, it is questionable whether a representation of information by a single probability distribution is justified from a scientific and methodological viewpoint.

In the previous chapter it was reminded how little-known information could be represented by a simple [min-max] interval, with limits defined, e.g., by expert judgment (**Figure 2**). However, oftentimes an expert is not only able to provide the boundaries of an interval, but also to express preferences within that interval. For example by specifying that values, e.g., in the middle of the interval, or close to the lower (or upper) limit, are more plausible than others. Possibility theory (Zadeh, 1978; Dudois et Prade, 1988) provides a mathematical framework for formalizing this type of information in a way that is analogous to the notion of imprecise probabilities illustrated in **Figure 15b**.

We consider the example of a rather poorly defined parameter: the Attenuation Factor (AF), used in the context of vapour intrusion into buildings. This AF factor is defined as the ratio of pollutant concentration in indoor air versus concentration in soil vapour in the immediate vicinity of the building. For a given pollutant concentration in soil gas, the higher the AF value, the higher the pollutant concentration in indoor air. While this is a generally poorly known parameter, there is nevertheless data published by USEPA from many sites in the United States (which were included in the FLUXOBAT project; Traverse et al., 2013). In France, the work of Derycke et al. (2018) on data collected as part of the so-called "Sensitive Facilities" programme, show that AF values depend, in addition to the nature of the pollutant, on various parameters such as the age of buildings: the AF is higher in the case of older buildings (slabs are more porous and therefore vapours penetrate them more easily). For a given situation and considering the "epistemic" nature of uncertainty related to this parameter, an expert might recommend:

- an interval of values he/she is certain to contain the value of AF;
- an interval of values (or a single value) he/she considers more likely than others.

Such information can be represented by a so-called “possibility distribution” (**Figure 16**), which associates (nested) intervals of parameter AF values with a measure of possibility (usually noted μ). For a given interval, called an "alpha-cut," 1 - μ is a lower limit of the probability that the value will be located in the interval. Thus, for the support of the distribution (the interval [2 x 10^{-4}; 6 x 10^{-4}]), we have: 1 - 0 = 1; i.e. it is certain that the value is included in the support (the probability is between 1 and 1). For the core, on the other hand: 1 - 1 = 0; i.e., it is not at all certain that the value is equal to the core (the probability is between 0 and 1). **Figure 17a** and **b** illustrate how the information contained in **Figure 16** translates into a family of cumulative probability distributions; i.e., all the distributions located between the upper limit (called Possibility; or Plausibility, Pl in Shafer's Belief Functions Theory, 1976) and the lower limit (called Necessity; N or Credibility; Cr; Shafer).

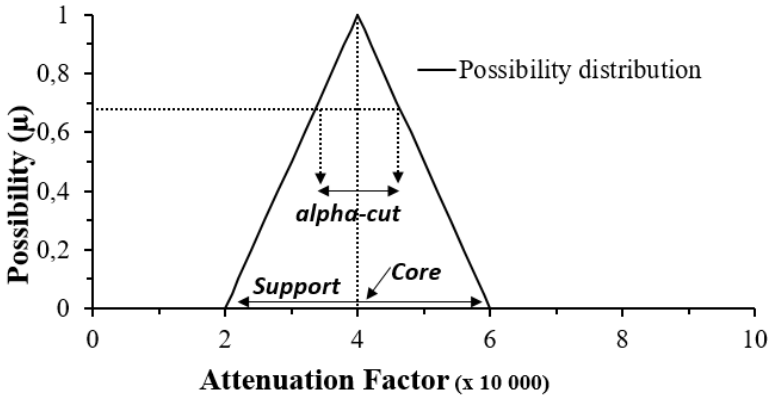

Figure 16 - Triangular possibility distribution for an expert judgment on the value of an attenuation factor.

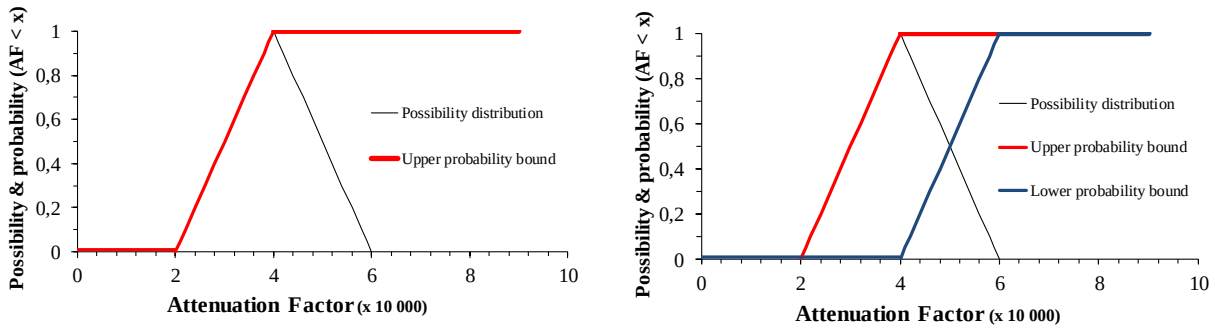

Figure 17 – Correspondence between the possibility distribution and a family of cumulative probability distributions.

This type of nested interval is particularly well suited for representing expert judgment, because an expert is generally consistent with himself: the interval of values he/she considers to be the most likely will necessarily be included within the range of values that he/she considers possible.

A "disadvantage" of this approach in the context of decision-making is that the incompleteness of the information is retained in the analysis (see section 2.5.2). While some researchers recommend using so-called "subjective" or "*a priori*" single probability distributions, with reference to a Bayesian framework (Lindley, 1971), many researchers (see e.g. Lloyd and Ries, 2007) question this approach when it is carried out in a context where no new data allows an “update” of the *a priori* distributions (using Bayes' theorem of conditional probabilities). In this case, the subjective Bayesian approach introduces a confusion between random variability and partial ignorance.

2.4.2. Uncertainty and spatial data

Uncertainties in spatial information are of different types:

- associated with the results of concentration measurements (e.g., measurement errors in the broadest sense, indirect measurements such as X-ray fluorescence for metals or photoionization detectors for organic compounds, measurements on portions of a drill core, etc.);
- inherent to maps derived from these measurements using an algorithm;
- linked to information regarding the medium, such as the thickness of a backfill (unknown or greater than the depth reached by the drill hole), the depth reached by the contamination, the topographical level of all or a portion of a site, the geological formations present in the subsurface and their position or limits, etc.

The first case is discussed here, while the following are addressed in section 2.4.8. The representation of concentration data can be statistical or spatial (using a map). Even when concentration data can be assumed to be "accurate", i.e., in the absence of measurement errors, their statistical summary may not be representative of values throughout the study area. Indeed:

- the study area might not be homogeneous in terms of the measured parameter (as when contamination is located in only one part of the site, or in a single type of backfill or soil material);
- the investigation might be biased (guided by site history), favouring high or low concentration levels;
- due to spatial correlation, local over-sampling may bias the distribution of data (the histogram) because closely-spaced values tend to be similar; particularly in terms of average and variance. This can be corrected by weighting the data according to the local density of the sampling investigation;
- in the case of variable-support data (e.g., variable core or analysed lengths), the concentration data population is no longer statistically homogeneous because variability depends on the support of the data. In this case the dispersion characteristics of the data (variance and coefficient of variation, quantiles, etc.) no longer reflect those of the true concentrations for a given support.

In the case of an analysis limit of quantification (LOQ), the limit (or limits) should be specified. The number of values that lie below the LOQ is an important piece of information. The influence of this number and of the LOQ values on the statistical analysis is easily assessed by successively setting the unquantified values to 0 and then to the LOQ. Unquantified values can also be made visible in maps by a specific symbol or colour, or by colouring all the associated on the histogram of the variable.

Duplicates (replicates) are useful for quantifying and visualizing measurement uncertainty (but certain assumptions are not always verifiable; de Fouquet, 2016). The dispersion of measurements appears on the data maps by simply superimposing symbols (circles, squares, triangles, etc.). When measurements can be divided into batches (e.g. 1st and 2nd subsample, or from two measuring devices), simple and bivariate statistical analysis of these batches (with correlation clouds, histogram superposition, difference statistics) can help detect the presence of a possible systematic deviation (bias) and provide the magnitude of measurement error variance. Simple and crossed sample variograms[3] of batch data are used to test certain statistical calculation hypotheses and to clarify the results (Chilès and Delfiner, 1999).

For the subsequent analyses (geostatistical analyses for establishing maps), it is preferable to keep the different measured values (replicates) rather than to use averages, in order to preserve information on measurement uncertainty (in the broad sense).

In the case when direct measurements of concentration (more reliable but more expensive) and indirect measurements (in larger numbers since they are less expensive, but also less reliable) are available, the statistical exploratory analysis (correlation clouds, empirical regressions) and variogram analysis (simple and crossed sample variograms) provide information on the relations between the two types of measurements. This is provided that there is a sufficient number of common measurement points

[3] The variogram represents, up to a factor 1/2, the average of the quadratic difference between two values as a function of their distance, taking into account orientation. The cross-variogram is, also up to a factor 1/2, the average of the product of the differences between two variables (the covariance of their increases) as a function of their distance, taking into account orientation.

(especially for the calculation of variograms) and that the two statistical populations are sampled. For subsequent mapping, the "transformation" of covariates into concentrations (using, e.g., linear regressions) should be avoided, as the concentration and the transformed covariable generally do not have the same variability.

The statistical or map representations of the data, supplemented by the exploratory and variogram analyses, allow a representation of data uncertainties and even a quantification if there is a sufficient number of replicates or different measurements at the same experimental points. This redundancy, which may seem costly, is the only way to quantify the uncertainty on the measured data.

2.4.3. Criteria for choosing uncertain information representation methods

As illustrated above, different modes of information and associated uncertainty representation are suited to different types of information (random variables versus imprecise parameters, spatial or not, etc.) and there is no “one-size-fits-all” method. The chart in **Figure 18** proposes to put these two dimensions (type of uncertain information and representation mode) in relation, in an attempt to promote consistency between the two. In particular, the aim is to avoid "creating" information that in fact does not exist, as is the case when a single probability distribution is assumed to represent incomplete/imprecise information. This chart is only a draft and should be reworked to improve its operational character.

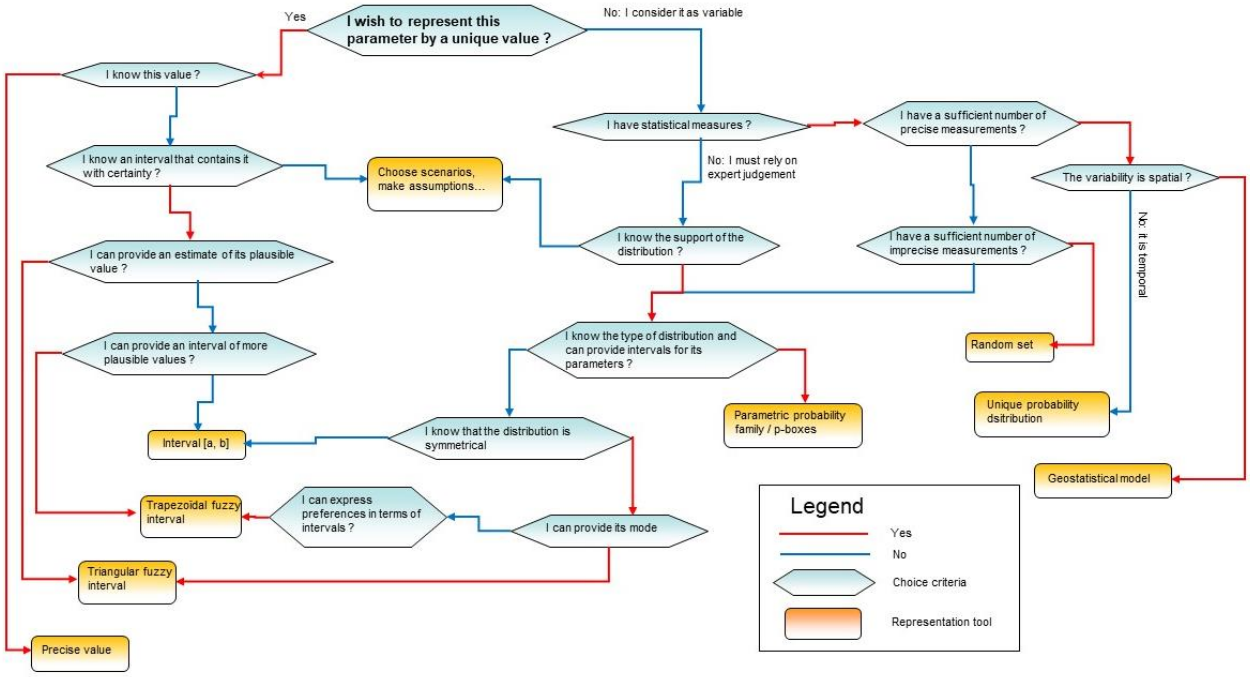

Figure 18 – A flow chart to link different types of information with representation methods (modified from Dubois and Guyonnet, 2011).

- Different types of information (precise, random, imprecise, spatial or not, etc.) warrant different modes of representation.
- Classical probability theory deals with random variables or functions, while the Bayesian approach can help address modelling uncertainty. Other information theories can be used to represent imprecise and/or incomplete information (e.g., possibility theory, belief functions, imprecise probabilities).
- The so-called "nested" intervals of possibility theory are particularly useful for representing expert judgment, where an expert expresses a range of values (support) in which he/she is certain to find the value of a parameter, as well as a value or interval of values within the support (core) which he/she considers most likely. These nested intervals result in "families" of probability distributions, as the information available is not sufficient to select only one.
- Spatial information is treated using geostatistics. Even when the data (e.g. soil concentrations) are assumed to be "precise", uncertainties remain due to the incomplete nature of investigations, heterogeneity of the study area, over-sampling in the presence of spatial correlation that alters the data distribution, etc.

2.4.4. Propagation of uncertainties in predictive models

Predictive models are used in contaminated land management to obtain estimates of future changes in environmental media quality (soil, air, water, etc.) or risks of health impacts, etc. Different types of models are selected based on objectives and context (see next section). To illustrate the propagation of uncertainties related to the model input parameters, we consider the generic situation where we have a risk calculation model (environmental or health) that is based on a number of parameters, noted X, Y, ..., Z. If uncertainty regarding these parameters can be represented by single probability distributions (because there is data to justify these distributions), then this uncertainty can be propagated through the model to the results using, for example, the well-known "Monte Carlo" method (see, e.g., Gobet, 2013).

The method is illustrated schematically in **Figure 19**. It consists in generating a random number (χ) for each uncertain parameter (in the event that the parameters are assumed to be statistically independent) and to "sample" the probability distributions at level χ of probability; i.e., finding the values x_i such that $P(X < x_i) = \chi$. The risk model calculation is performed using sampled values x_i, y_i, ... Repeating this procedure a large number of times, a representative sample of the risk model results is obtained and it is then possible to construct a cumulative relative frequency diagram for calculated risk. In practice, all calculated risk values are sorted in increasing order and each value is assigned a frequency of 1/n, where n is the number of iterations. If the number of iterations is sufficient, the cumulative frequency graph is taken as a cumulative probability distribution and specific quantiles can then be compared to the risk threshold to determine whether the calculated risk is acceptable or not.

It should be noted that because of the required computational effort, the Monte Carlo method applies mainly to so-called "analytical" models (mathematical solutions of equations describing the phenomena influencing risk) rather than to numerical models (methods using a discretized mesh; see next section).

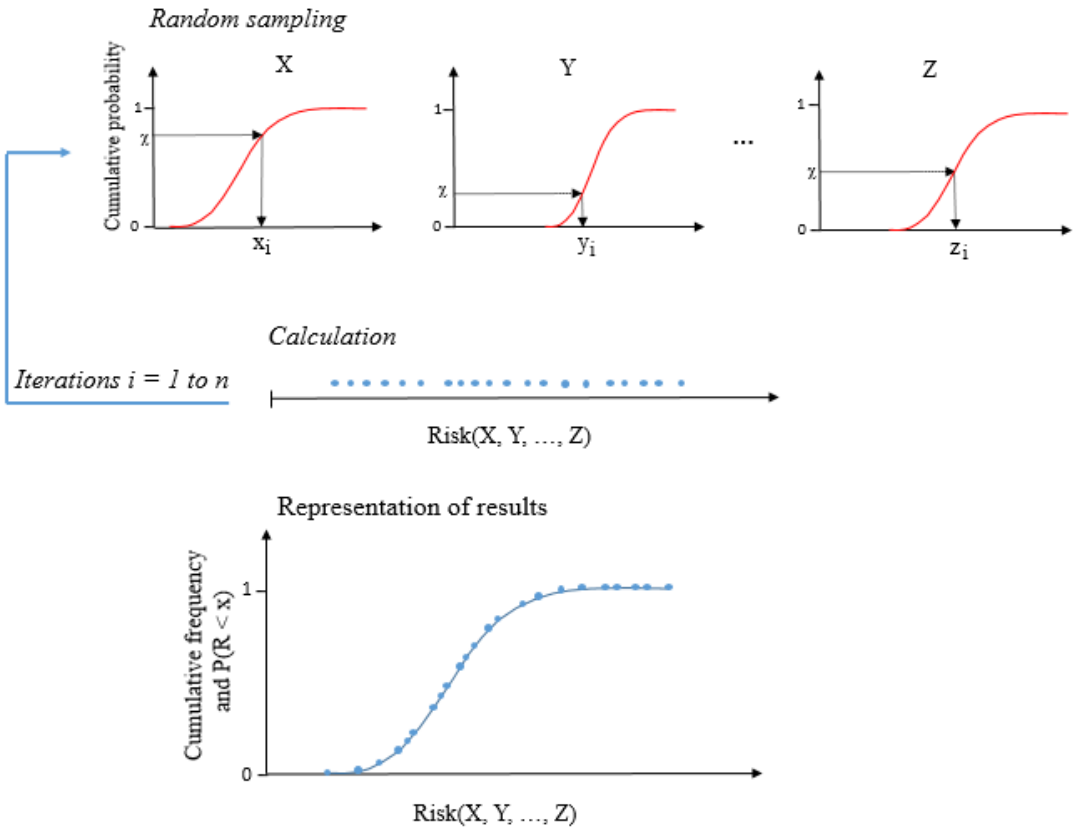

Figure 19 - A schematic illustration of the propagation of uncertainty in a risk model using the Monte Carlo method.

If one or more parameters are not represented by single probability distributions (for lack of information), but rather by one of the other representation tools illustrated in the previous section (probability families, intervals, nested or not ...), then we can proceed in a similar way, but instead of obtaining a single distribution for the result of the risk calculation, we obtain a family of distributions. This is illustrated in

Figure 20 for the simple case of a risk model for which all but one (Z) parameters are represented by single probability distributions, while for Z it is only known that its value lies somewhere between a value min and a value max (classical interval). In this case, the procedure consists (Baudrit et al., 2006), as in the classical Monte Carlo case, in randomly sampling the probability distributions, but this time all possible values of Z must be taken into account over the interval [Z_{min}; Z_{max}]. From an operational point of view, we can distinguish between two situations: (i) either the model is simple (monotone) and the min and max values of the risk calculation are obtained from the min and max values on Z, or (ii) the model is more complex and then an optimization algorithm is required to find the min and max values of the risk calculation by scanning over all the values on Z.

In both situations, the result of the calculation is what is called a "random interval." The corresponding probability distribution family is obtained by classifying all min values in ascending order, the same for all max values and assigning a relative frequency equal to 1/n (n is the number of iterations) to each [min, max] pair. This defines the lower (credibility; Cr, Shafer, 1976) and upper (plausibility; Pl, Shafer) probability bounds for the proposal "calculated risk is lower than a certain value"; P(R < x) in

Figure 20.

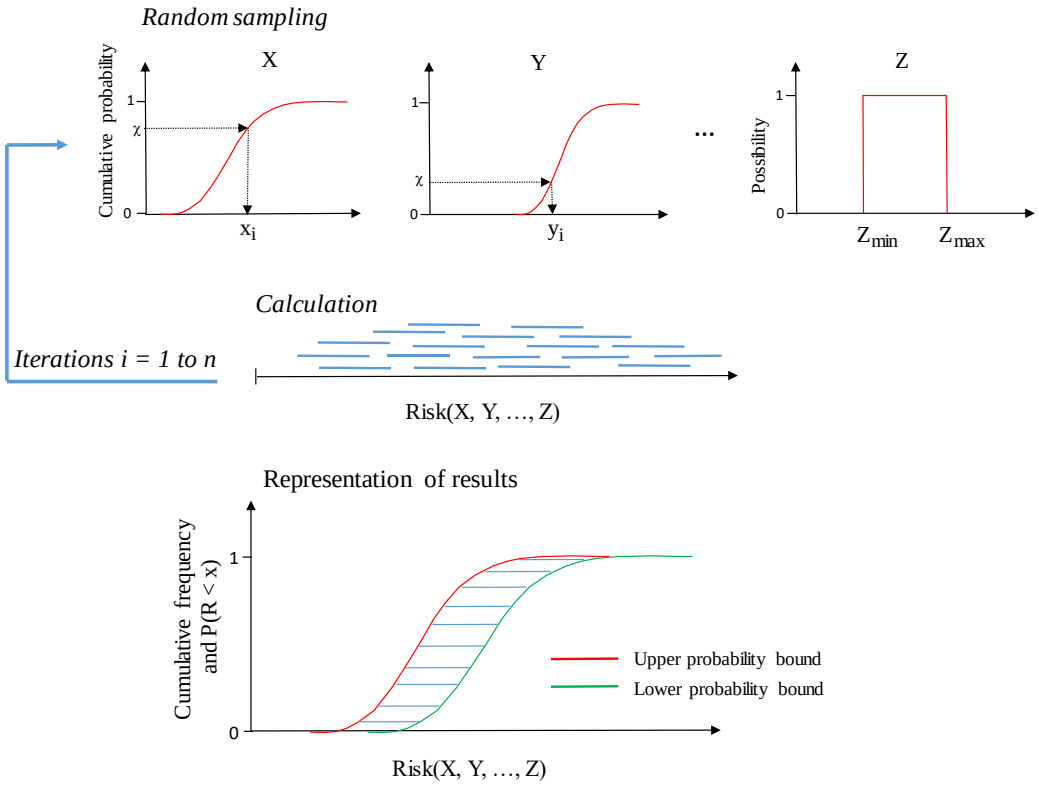

Figure 20 - Schematic illustration of the joint propagation of random and incomplete/imprecise information.

2.4.5. Uncertainties associated with predictive models

The previous section addressed the issue of uncertainties relative to predictive model parameters. But there is also the issue of uncertainty pertaining to the predictive model itself: conceptual model, way of representing underlying mechanisms, resolution algorithms, etc. In this case, one approach may be to use several models deemed "eligible" and to synthesize the results as previously illustrated, while possibly assigning different weights to the results of different models, depending on the level of confidence that one wishes to grant them.

a) The conceptual model

As specified by the French national methodology for managing contaminated land (DGPR, 2017), prior to performing an inventory of environmental media quality on a site or to developing a site management plan, a preliminary study should be performed in order to gather all available information regarding the site and summarized in the form of a conceptual model. This conceptual model aims to present, in a very synthetic way, the state of contamination of the environment and the possible modes of contamination in relation to activities and practices on the site and in its vicinity. An example of a conceptual model, for the case of contamination by a dense non-aqueous phase chlorinated organic compound (heavier than water; DNAPL), is presented in **Figure 21**.

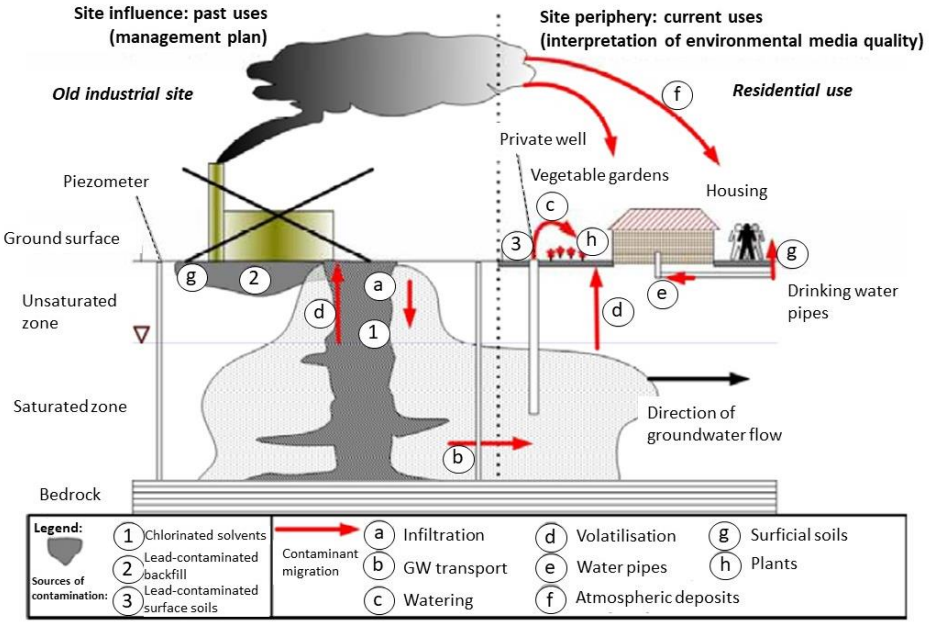

Figure 21 - Example of a conceptual model illustrating pollutant sources, transfer pathways, etc. (modified from: http://ssp-infoterre.brgm.fr/schema-conceptuel)

Of course, uncertainties also exist at the conceptual model building stage. For example and in reference to **Figure 21**, the groundwater flow direction might be poorly understood (due, e.g., to insufficient characterization of piezometer levels). Or the volumes of spilled DNAPL might be underestimated and therefore the duration of the "source term" or the volumes of soil to be remediated might be much larger than expected. There are also uncertainties regarding the physical and chemical mechanisms that influence the fate of pollutants in their different forms (pure phase, dissolved, gaseous, adsorbed, etc.).

But the development of the conceptual scheme is an opportunity to summarize what is known about a site and to highlight possible "areas of uncertainty" which might lead to further investigations, thus reducing uncertainty and increasing the relevance of future proposed management actions.

b) Analytical models

Analytical models are mathematical solutions to the equations that describe the phenomena influencing impacts and risks. In the case for example of the transfer of contaminants in the subsurface, they are solutions to the partial derivative equations that describe the fate of contaminants influenced by mechanisms such as transport by mobile water (advection), dispersion and diffusion, adsorption onto the solid phase, volatilization, etc. One of the significant advantages of analytical models is to avoid the numerical dispersion associated with mesh models (next section), which is another source of uncertainty. Another advantage is calculation speed compared with mesh models, especially in the case of transient problems (as there is no need to iterate in time). In view of this calculation speed, analytical models are particularly well suited to uncertainty analysis schemes, such as the Monte Carlo method (see section 2.4.4). But analytical solutions also have their disadvantages, which include the constraints in terms of simplified modelled domain geometries and boundary conditions. Despite their limitations, analytical models are very useful as a first computational approach, or to "verify" the results of numerical models.

There are many examples of applications of analytical models in the field of contaminated land. With respect to contaminant transport, there are for example analytical solutions applied to the biodegradation of pollutants in groundwater plumes (Hunkeler et al., 2010, Gutierrez et al., 2009), solutions for the 3-dimensional transport of solutes in groundwater and for various geometries (e.g., Guyonnet, 2008; **Figure 22**, Guyonnet and Neville, 2004) or semi-analytical approaches developed for example for pollutants influenced by redox phenomena (e.g., BTEX; Atteia and Huhener, 2012).

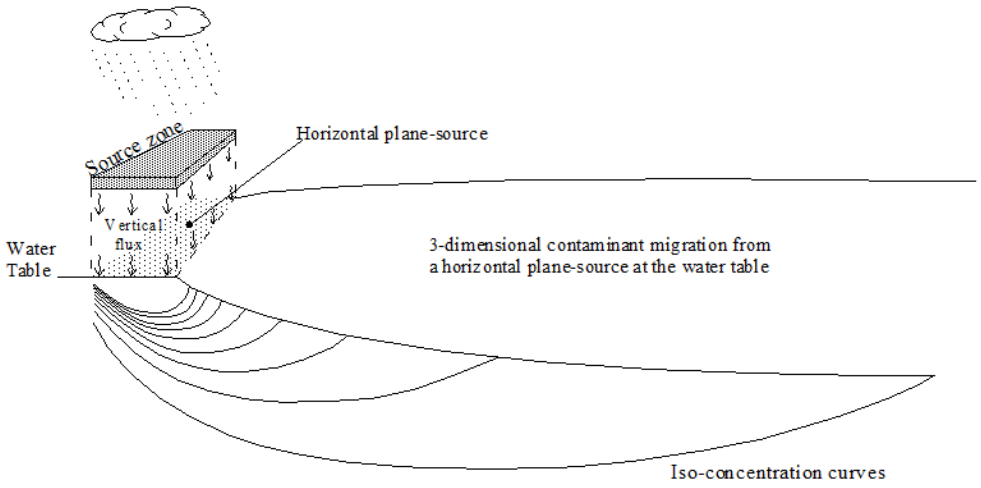

Figure 22 - Conceptual model of the MISP analytical model (Guyonnet, 2008)

c) Numerical models

In the field of contaminated land, possibly the most commonly used numerical models for simulating the migration of pollutants in groundwater are Visual MODFLOW (from Waterloo Hydrogeologic Inc.); **Figure 23**) and FEFLOW (from DHI Group). But there are many other numerical models, which address specific aspects of this field. For example, although it is less developed that the two previous models in terms of graphical capabilities, the MARTHE model developed by BRGM (Thiéry, 2014), has several advantages in terms of, e.g., numerical dispersion control.

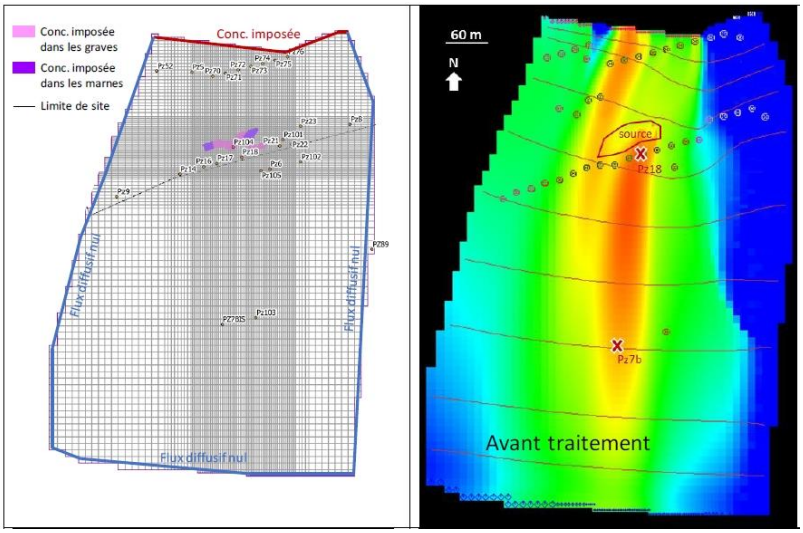

Figure 23 - Example of numerical modelling of contaminant (dichloroethylene) migration in groundwater using the Visual MODFLOW numerical model (Chastanet et al., 2019)

In terms of addressing uncertainties, the disadvantage of numerical mesh models is the computational time associated with one simulation. Indeed, when it is necessary to multiply the number of simulations in order to scan over ranges of possible parameter values, computational time can become prohibitive. In a study supported by ADEME, Chastanet et al. (2019) proposed to overcome this difficulty by using a "metamodel" that reproduces the behaviour of the complete numerical model but with much less computational time, and to treat uncertainties using the calibrated metamodel.

2.4.6. Comparing results from a predictive model to a precise threshold

Comparison between results of a predictive model and a precise threshold is illustrated in **Figure 24** for the two cases considered in section 2.4.4: the classical probabilistic representation (**Figure 24a**) and the hybrid case (**Figure 24b**). In case a), the threshold is often compared to a 90% or 95% quantile and the risk is considered acceptable if the threshold is higher than the corresponding risk values: the probability that the risk is lower than the threshold is at least 90%. In case (b), the situation is less trivial because the comparison with a threshold provides two values: an upper and a lower probability bound. In the case of **Figure 24b**, the probability that the calculated risk lies below the threshold is between 0.95 (Plausibility; Pl) and 0.6 (Credibility; Cr). The section on stakeholder communication (section 2.5) examines how to address this type of result.

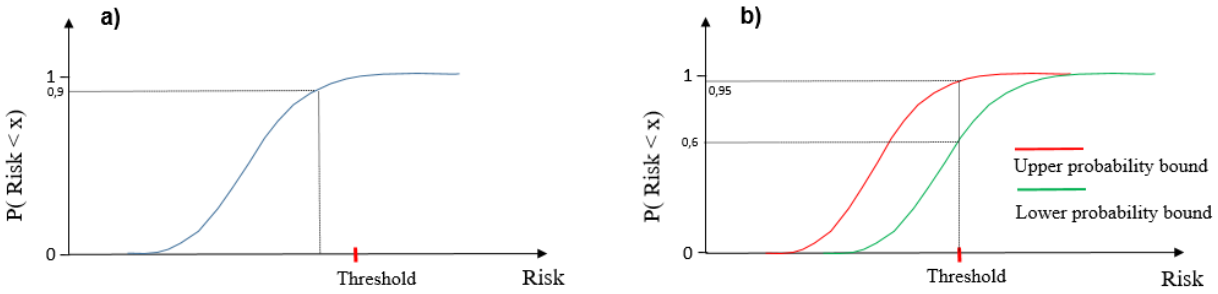

Figure 24 - Comparison of a risk calculation result to a precise risk threshold.

2.4.7. Comparison with an imprecise threshold

Considering the uncertainties associated with determining risk thresholds, it may seem surprising that such thresholds are represented, in the extreme majority of cases, by precise values. But as shown by several authors, this is not mandatory. For example, in an analysis of the health risks induced by nitrate consumption, Lee et al. (1994) used a "fuzzy" threshold to define an acceptable Danger Quotient (DQ), illustrated in **Figure 25**. For a value DQ < 1, appearance of methemoglobinemia among people exposed to nitrate consumption is not expected, unlike when DQ > 1.5. Between these two values, methemoglobinemia is considered possible, with a degree of possibility that varies linearly in first approximation.

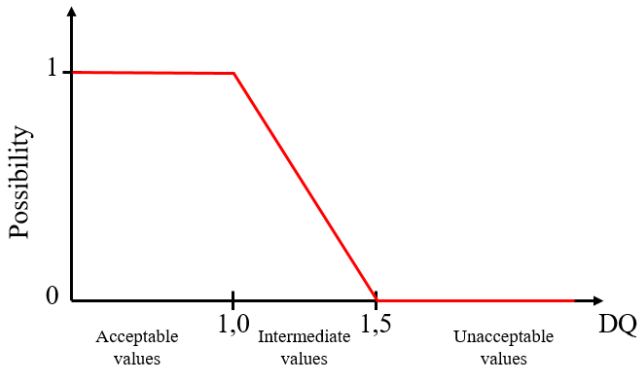

Figure 25 – Fuzzy acceptability threshold for a danger quotient; DQ.

This type of representation (offering a gradual transition between what would appear totally acceptable and what is unacceptable) could be applied to thresholds in other situations, where the use of "yes-no thresholds" may generate difficulties in terms of site management. In the case of **Figure 25**, it would be up to the decision-maker to specify which degree of possibility is required to establish the acceptability of the calculated Danger Quotient (see Como et al., 1997). Similar thinking could be applied to the development of toxicological values used in risk analysis. For example for establishing values of PNECs (predicted no-

effect concentrations) or RTVs (reference toxicological values) which, despite the use of so-called "uncertainty factors", are typically represented by precise values.

This method of representation could be applied to urban pedogeochemical backgrounds, the definition of which may have significant consequences for the management of contaminated land (e.g., for selecting the destination of excavated soils) and thus help to identify soil concentrations that highlight anomalies versus concentrations that are representative of a pedogeochemical background (anthropized or not). Considering the significant uncertainties involved in the definition of such backgrounds (Sauvaget, 2019), the use of precise thresholds may sometimes be questionable and a representation such as in **Figure 26** might seem more appropriate. Given that in urban areas, all soils are more or less influenced by anthropogenic activity (we have entered the Anthropocene era...), the scientific definition of the very concept of urban pedogeochemical background is up to discussion (see section 2.4.8). Indeed, it might be more appropriate to speak of a "soil-concentration anomaly reference base", to help with decisions in terms of management actions.

Finally, it should be reminded that in a given geographical area, the proportion of concentrations exceeding a fixed threshold depends on the measurement support, i.e,. the geometry (and hence volume) of the medium sampled (a whole core, part of a core, etc.; see section 2.4.8). A concentration threshold should therefore be associated with information on the corresponding support (e.g., litre, m^3 or 10 m^3, etc.).

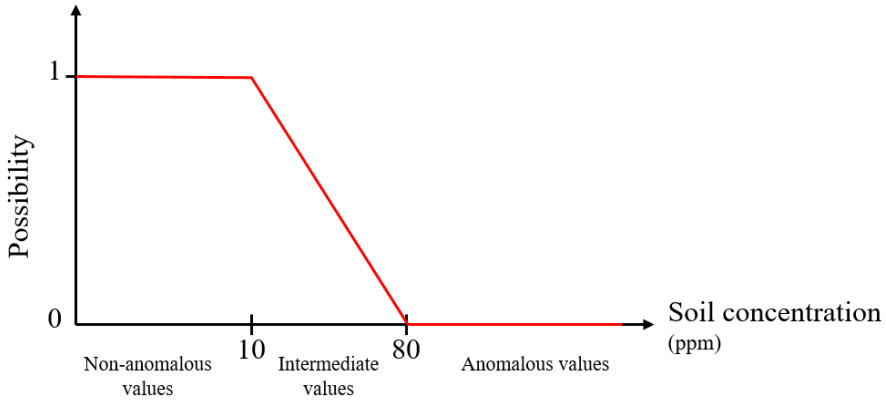

Figure 26 - Fuzzy urban pedogeochemical background.

- Imprecise information can be propagated through a risk calculation model, in addition to stochastic information.
- A practical method combines the well-known "Monte Carlo" method with a search for [min - max] bounds.
- The results can be compared to thresholds that may be precise (the general case) but also imprecise.

2.4.8. Use of spatial data

The use of concentration maps calculated from very scarce information is first examined by introducing a distinction between the case of a single contaminated site from that of the evaluation of an anthropized pedogeochemical background, the definition of which is not yet definitive (see previous discussion). The case of imprecise measurements is then examined, with particular reference to indirect investigations (e.g.,

geophysical) where numerous albeit imprecise data are collected, and to a context of remediation via soil excavation. The concept of "support" of an estimation is finally discussed.

a) Drafting and using a site concentration map

Regardless of the remediation process, its implementation at large sites requires one or more concentration maps (organic compounds or families of compounds, metallic elements, etc.). The data collected are concentration measurements, possibly supplemented by the description of soil formations. Because concentrations are not known exhaustively (neither at the surface nor at depth), the areas to be remediated are therefore delineated based on an interpolated or estimated result, and not from an "exact" concentration map.

- **Reminder on interpolation or estimation methods**

An estimate is said to be linear if the calculated value is a linear combination (a weighted average) of the data. Noting concentration as “z” and x_i for data coordinates (e.g., at the centre of a core), the estimated concentration at point x is written: $z^*(x) = \sum_i \ \ell_i \, z(x_i)$, where the star indicates that it is an estimate, not the true value. Interpolation methods (nearest-neighbour estimates, weighting by an inverse distance power, for example) are based on the intuitive assumption that concentrations in two samples taken at points close to each other, should be similar. As a result, the weights assigned to the data closest to the point or block to be estimated are higher.

Among existing interpolation methods, kriging is the optimal linear estimator in the sense that, in the explicit probabilistic model, the estimate is unbiased and the variance of the estimation error is minimal. Rather than being determined by the sole geometry of the data and points to be estimated, the kriging weights depend (i) on the support of the variable to be estimated ("point" average on a mesh of given geometry, …) and on the support of the data, as well as (ii) the spatial variability of the considered variable. For a given data geometry and "target" to be estimated, the weights will differ depending on the relative spatial regularity of the variable.

Spatial variability is quantified using the variogram, which reflects the variability of the concentration at two-points as a function of their distance (**Figure 27**). Complementary variographic tools (clouds and variographic maps) are useful for detecting anomalies and possible preferential directions (anisotropy). The sample variogram is calculated from the data and then fitted by a model summarizing the main characteristics of the spatial variability.

When data are scarce, the experimental variogram, available for a few distances and directions, may differ significantly from the hypothetical "complete" variogram, which would be calculated if all concentrations in the study area were known. The cross-validation technique can help in selecting the variogram model that will be used for kriging. An analysis of the sensitivity of estimation results to the adjusted model is a simplified way to account for modelling uncertainty.

Different techniques enable to specify the spatial structure despite an "erratic" variogram, assuming there is a sufficient amount of data available. Useful for clarifying spatial variability, data transformations require specific modelling techniques (anamorphosis and estimation by disjunctive kriging or conditional expectation), in order to avoid estimation biases.

There are many variants of kriging, depending on whether the estimate is mono-variable or multi-variable (several concentrations simultaneously, or taking into account co-variables to improve accuracy). Specific models, such as the top-cut model (Rivoirard et al.; Donati et al.,2018) have been developed to address problems posed by very high values in the data.

The kriging method also provides a map of the standard deviation (the square root of the variance) of the estimation-error, which can be corrected to account for the proportionality effect (which often occurs): spatial variability depends on the local average of concentration and generally increases with it (this correction was applied for **Figure 28**).

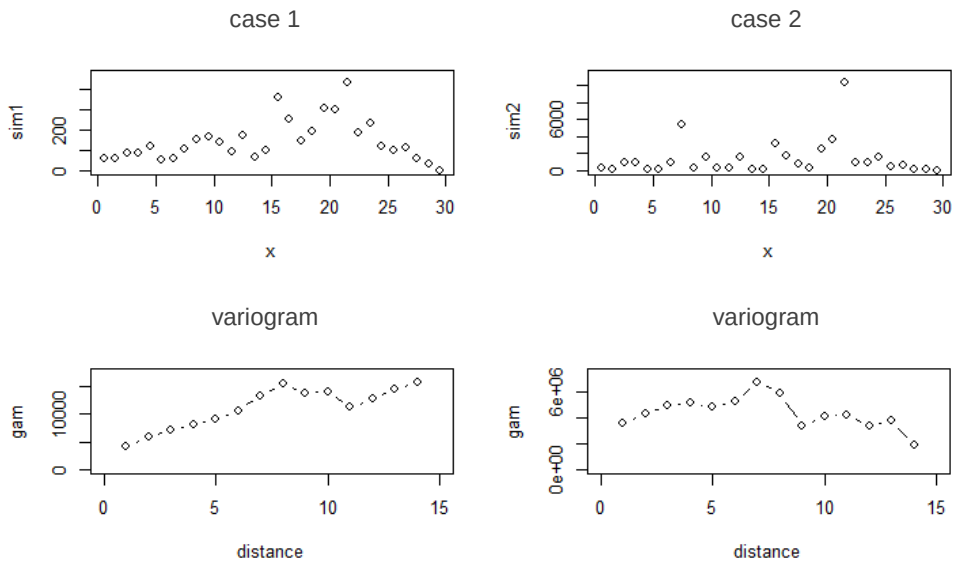

Figure 27 - Two concentration transects (top) and their respective variograms (bottom).

Note: The greater irregularity of case 2 compared to case 1 is reflected in the amplitude of the variogram (10^6 versus 10^4), its greater discontinuity relative to the origin, and its shorter range.

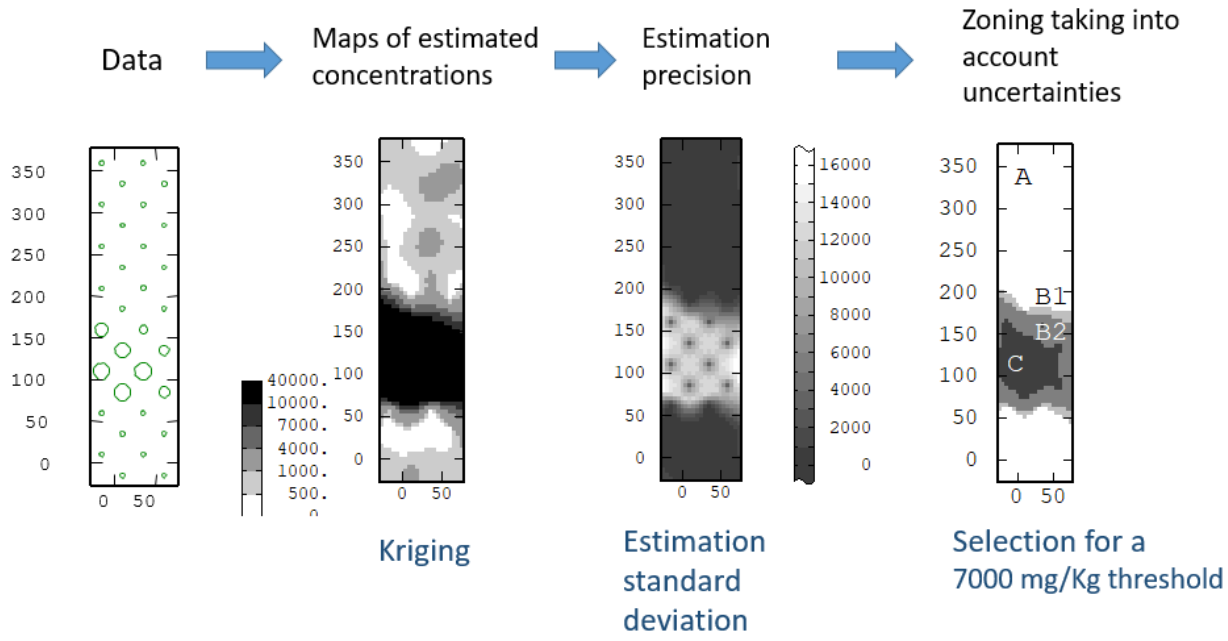

Figure 28 – From the data to the map of spatial variability (LOQUAS project, Benoit et al., 2010).

Converting the error-estimation standard deviation into a probability interval requires a hypothesis regarding the error histogram. Non-linear estimators (disjunctive kriging, conditional expectation) were designed to answer this question in a rigorous fashion. These methods are not often used in the context of contaminated land management, for several reasons: (i) consulting companies typically have strict time constraints and often lack expertise in geostatistics and (ii) the hypotheses on which these "advanced" methods are based are not always experimentally verified for a given situation, which requires adapting them to the situation at

hand. In practice, an approximate solution could be empirically deduced from the study of the standardized error (i.e. the error reported to its kriging standard deviation), obtained by cross-validation; but the validity of such approximations is to be considered carefully.

- **Selecting based on the estimated concentration map?**

The delineation of areas where the concentration exceeds a fixed threshold s must take into account the estimation error. In fact, selecting from the estimated concentrations is analogous to selecting blocks v_i whose estimated concentration values exceed the threshold s, which can be written: $z^*(v_i) \geq s$. As the concentration is the sum of its estimate and the associated error estimate; $r(v_i)$, $z(v_i) = z^*(v_i) + r(v_i)$, blocks whose actual concentration exceeds the threshold are such that: $z(v_i) \geq s$, i.e., $z^*(v_i) \geq s - r(v_i)$, where the estimation error $r(v_i)$ is unknown, but for which the geostatistical model specifies that the (probabilistic) average is zero and that the variance is the kriging variance. Using a hypothesis on the histogram of the standardized error, one can choose (with a statistical risk) the quantiles q_ζ (negative and noted $-|q_\zeta|$ below) and q_η (positive) of the standardized error defining an interval (not necessarily symmetrical) around the estimated value $z^*(v_i)$, interval to which the unknown true value has, in the model, a high probability of belonging. Noting $\sigma_k(v_i)$ the kriging standard deviation, with a fixed statistical risk, we have the estimated concentration: $z^*(v_i) - |q_\zeta|\sigma_K(v_i) \leq z(v_i) \leq z^*(v_i) + q_\eta\sigma_K(v_i)$. A comparison of the boundaries of this interval with the threshold s, highlights three cases (Cori , 2005):

- $s \leq z^*(v_i) - |q_\zeta|\,\sigma_K(v_i)$; the threshold is lower than the lower bound of the interval: the block is located within the contaminated area;
- $z^*(v_i) + q_\eta\sigma_K(v_i) \leq s$; the threshold is higher than the upper bound of the interval: the block is not contaminated;
- $z^*(v_i) - |q_\zeta|\sigma_K(v_i) \leq s \leq z^*(v_i) + q_\eta\sigma_K(v_i)$; the threshold belongs to the probability interval: because of the estimation uncertainty, it is not possible to know whether the block is contaminated or not. The block belongs to the zone of uncertainty (**Figure 28**).

Depending on the size of the uncertainty zone, it may be useful to specify two portions (noted B1 and B2 in **Figure 28**) depending on whether the concentration is below or above the threshold. If it is technically possible (delays, costs), additional investigations should be focused within and on the (external) periphery of this area.

Non-linear estimators (conditional expectation and uniform conditioning within the transformed Gaussian model, disjunctive kriging) which provide a rigorous estimate of local distribution (of the local histogram), allow such calculations. However, the hypotheses of the most conventional model (the transformed Gaussian model) are not always verified, especially in the case of substances whose concentrations are strongly dispersed, as is the case for certain organic contaminants. The research must therefore be continued.

In practice, it is useful to improve the accuracy of estimates, for example by taking into account more numerous albeit less precise indirect measurements. But the "experimental points" common to both types of measurements (direct and indirect) must be in sufficient numbers to allow the analysis of the correlation between the two types of measurements (comparison of averages and averages by concentration classes), as well as the fitting of a bivariate variogram model.

- **Regarding the change-of-support issue**

As mentioned above, the delineation of the contaminated area depends on the support of the selected unit, which is rarely specified. Spatial support means the shape, size, and orientation of the considered unit (core, block...). The proportion of drill cores with a concentration above the threshold s, differs from that of "small" blocks (e.g. 2.5m x 2.5m x 1.5m) exceeding this threshold, which is itself different from that of "large" blocks (e.g. 10m x 10m x 3m, or 32 times larger) above the threshold. The support affects the order of magnitude of the results.

The selected support should therefore be specified at the same time as the threshold s. This needs to be taken into account especially in the event of post-remediation control, if the concentration of the "control" sample exceeds the threshold. Non-linear geostatistical estimators can calculate the "*probability that the*

concentration in a block should exceed the threshold, knowing the concentration of a sample in the block". In practice, the influence of the support is bypassed by the choice of the threshold, which depends more or less on the context.

b) Urban geochemical background: what definition?

The pedogeochemical background in a degraded environment is generally calculated using statistical criteria developed for the detection of anomalies: higher-order quantiles (90 or 95%), criteria constructed as the sum of a central value and a dispersion indicator (upper whisker, deviation from the median). By default, concentrations below the selected criterion are assumed to correspond to the "background".

This calculation has several drawbacks: the common statistical calculation does not take into account the location of the data, nor the spatial correlation between variables. Moreover, how is its parameterization justified? For example, are the criteria calculated using all the data in the study area, or using neighbourhood criteria, and in this case, how is this neighbourhood determined? How is the available information regarding the degraded environment taken into account (current and historical land use, geological nature of the substrate, etc.)?

Provided certain assumptions, the statistical criteria follow a partial order (Sauvaget, 2019), but these assumptions are not necessarily verified (e.g., symmetrical or weakly dispersed distributions). The choice of a single statistical criterion is therefore likely to be empirical.

Another approach is to define the anthropized pedogeochemical background based on the different scales of contaminant variability in the studied area, using kriging analysis, also known as "factorial kriging" (Sauvaget, 2019). The decomposition of the variable into scale components is based on a variographic analysis, and may take into account the co-variables describing the degraded environment. The results depend on the studied area, which is to be expected: an anomaly over a large area might be partially seen as an "anthropized background" over a smaller area which is completely under the influence of a source of contamination. This highlights the uncertainty associated with the definition of the size of the studied area.

The calculation, by kriging analysis, of a map of the background and anomalies requires specifying to which component the "average" of the studied variable should be associated, which introduces an indeterminacy in the result. Depending on the modelling choice, the "anomalies" can thus be of zero average (in the model). Different definitions of background and anomalies, which differ locally by a constant (the value of which changes with the neighbourhood) are therefore possible. The interpretation of this indeterminacy deserves additional research, in order to help justify the obtained maps.

Finally, the use of the resulting maps is a topic that would require additional discussion:

- choice of the mesh and of the support: estimation of a “point-value” (at the node of the grid), or of a spatial average (regularized value). One could even consider a larger support for the estimation of the “background” than for the “anomalies”;
- for the background, should we consider a local maximum (and in this case, in which neighbourhood?) of the estimated values?
- how to account for the estimation-error variances of the background and anomalies, provided by the kriging analysis, variances that depend on the location of the sampling points, the estimated mesh and on the variogram (or simple and cross-variograms of the variable and covariates)?

- The study of a contaminated site requires “sufficient” concentration data. An initial phase of data quality analysis and sorting is useful. The geostatistical exploratory analysis enhances the study through a synthetic description of the spatial distribution of concentration. Geostatistical estimators (kriging and variations thereof) improve the accuracy of maps, but do not compensate for lack of data and/or their insufficient quality. Inadequate site investigation generates uncertainties that are not necessarily identified.
- Rapid (indirect) on-site measurements can improve the accuracy of estimates at a small cost, provided that there is good correlation between direct and indirect measurements and sufficient common measurement points. Taking into account co-variables such as soil formations improves estimates, but requires detailed preliminary analysis.
- The delineation of the areas to be remediated must take into account estimation uncertainties and therefore cannot be carried out directly based on the map of the estimated concentrations. Different methods for comparing estimated concentrations to a threshold are available. However, they are seldom used, due to the time constraints which consulting companies must deal with and because these methods require expertise in geostatistics, especially in complex cases.
- The determination of a clean-up threshold should specify the associated "support" (the volume to which the concentration value refers). In practice, reference to the support is generally bypassed by the choice of the threshold, which is more or less high depending on the context of the site.

2.5. Decision and communication

2.5.1. A multi-partner approach

Approaches for addressing and communicating uncertainties in a context of contaminated land management are generally primarily technical and computational. But more "partnership-based" approaches can also be considered, in order to draw from the "collective intelligence". Indeed, in a review of the involvement of different stakeholders in contaminated land management (INERIS-IRSN, 2008), it was shown how such involvement may significantly improve the management process, despite inherent uncertainties and thanks to a better shared understanding of issues.

In a study conducted for ADEME, Hazebrouck et al. (2008) propose methods and tools for communicating in a context of contaminated land management, that are also suitable for other types of environmental risks (cf. COMRISK platform; https://comrisk.fr). Multi-partner approaches to urban brownfield management have also been proposed by the Baltic Urban Lab (2018). These examples emphasize that the manner in which risks and associated uncertainties are represented must necessarily take into account the identity of the stakeholders receiving the information. Indeed, in a sociological study carried out on the basis of questionnaires and interviews with populations suffering from air pollution, Harpet et al. (2005) conclude that: "*communicating on uncertainties with people who are "certain" of being victims, is simply not an option...* ». In such a context, a prerequisite to communication with non-technical stakeholders would be the sharing of a common language, understood by all in terms of vocabulary, formulations, images, concepts, etc.

In addition to information regarding ongoing studies (via letters, public meetings, etc.), it appears more and more necessary to organize work meetings with stakeholders (including local residents), ahead of the actual studies or works, in order to present and discuss the selected approaches, hypotheses, etc. and only at a later stage to discuss results and knowledge limitations.

2.5.2. Communicating on epistemic uncertainties

Communication between and with stakeholders of contaminated land, be it the managers of the land (owners, operators, developers, ...), regulatory bodies (local, national, etc.), civil society (representatives of local communities, associations, residents, ...) etc., is an essential aspect of contaminated land management. With respect to the communication on uncertainties, experience shows that it is already difficult to communicate on the risk of exceeding thresholds expressed in a conventional probabilistic framework (using single probability distributions). We can therefore expect even more difficulties when it comes to communicating on *imprecise* probabilities of exceeding thresholds... (in the case of epistemic uncertainties).

To overcome this difficulty, we can draw from the experience in the field of meteorology, where scientists rely on a large number of measurements to make forecasts and communicate them to a very wide audience. A significant difference with the field of contaminated land is the fact that meteorologists have rapid feedback on the reliability of their forecasts, whereas for contaminated land, where mechanisms are comparatively much slower, feedback on forecasts is often obtained only after many years. However, it is very instructive to examine how this community communicates about uncertainties, as it can be recognized that compared to the community of contaminated land management, meteorologists are particularly experienced in terms of communication.

Meteorologists rely on so-called "ensemble forecasting" (Palmer et al., 2005), which consists in calculating global atmospheric flows from several initial states deemed "plausible." The results of these forecasts are accompanied by a reliability estimator that is not dubbed "probability" (a term that implies a certain completeness of the exploration of alternatives), but rather "confidence index". Note that this term, much more flexible than the term “probability”, seems to be well received by the public with which meteorologists frequently communicate (news, radio, press, etc.). The confidence index, typically a value between 1 and 5, provides the public with a qualitative estimate of the reliability of the forecast (5 = very reliable, 1 = unreliable, ...). The public that is provided a forecast with a "confidence index" does not need to know the mathematical details underlying its development: it is sufficient for the public to know whether the expert is confident or not in his forecast.

Based on this example, Dubois and Guyonnet (2011) used the concept of a confidence index to propose a single estimator of the degree to which a threshold (accurate or not) is exceeded. Drawing on the work of Hurwicz (1951), they propose to calculate a confidence index (IC) from a weighted average of the upper and lower probability bounds in **Figure 24b**:

$$IC = \alpha\ Pl + (1- \alpha)\ Cr$$

Where α is a weighting factor.

A value of 0 is tantamount to assuming IC = Cr: the most pessimistic indicator is taken, which may seem overly conservative, since all available information suggesting a less severe risk is ignored. A value of 1 is tantamount to assuming IC = Pl, which is overly optimistic; i.e., non-conservative and therefore difficult to justify in a context of contaminated land management, where there is an attitude of “aversion to risk”. It has been proposed conventionally to set α at a value of 1/3, which implies that a weight of 1/3 is given to the optimistic bound, and 2/3 to the pessimistic bound. It is suggested that this approach helps define a single "reasonably conservative" indicator of the degree of exceeding the threshold. This index is illustrated in **Figure 29**.

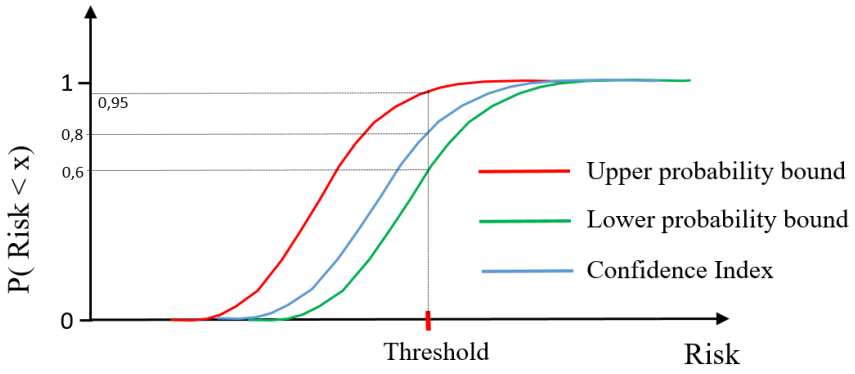

Figure 29 - Family of probability distributions and confidence index.

One might object that this approach introduces a component of subjectivity, whereas the criticism previously formulated in relation to the "Bayesian" approach was precisely related to its subjective character. But here subjectivity is introduced at a decision-making stage, not upstream of the risk calculation by confusing random variability with lack of information, which is the case when single probability distributions are "stipulated" without justification by data.

When dealing with incomplete/imprecise sources of information, the restitution of a risk estimate in the form of a family of probability distributions, such as the one schematically represented in **Figure 29**, presents the advantage of illustrating the range of possible values of risk. The distance between the upper and lower probability bounds in **Figure 29** directly reflects our lack of knowledge regarding certain parameters influencing the risk. If this distance is deemed too large, it might be decided to reduce it by improving knowledge (by measurement) of a particular parameter of influence (a sensitivity analysis can help identify the most influential parameters). Such a choice cannot result, on the other hand, from an analysis where it is arbitrarily decided to represent poorly-known parameters by single probability distributions (e.g. uniform distributions), as there is then no way to distinguish, in the variability of the calculated result, what results from true random variability versus information incompleteness (Dubois and Guyonnet , 2011).

Note that while the threshold in **Figure 29** is "precise", the same comparison exercise could be done in the case of a "fuzzy" threshold (see **Figure 25**). The latter could be tested in practice, in particular to determine whether it represents added-value in terms of flexibility compared to the precise threshold case. Indeed, it is common in practice that a slight threshold overshoot on one or two parameters may call into question a management option. But if we consider all the uncertainties associated with the development of certain thresholds (for, e.g., health risks), the use of transition zones between what seems totally acceptable and what is not at all acceptable, may seem justified.

- Taking into account the incomplete/imprecise nature of the information available allows for communication on the extent of the results considered plausible.
- For comparison between results and an acceptability threshold (precise or imprecise), a single indicator can be used (here called a "confidence index").
- Considering the many uncertainties affecting the definition of acceptability thresholds, the use of imprecise risk thresholds is worth exploring.
- Risk communication cannot be limited to technical and/or computational approaches: sociological and partnership approaches, drawing from the collective intelligence, are also necessary.

2.6. Management measures and monitoring

Management measures for contaminated land are varied and include the excavation of contaminated soil, clean-up, safety measures, monitoring of environmental media, etc., phases during which new data is collected. Among the main stakeholders to be impacted directly (especially financially) by uncertainties are the consulting companies in charge of implementing management measures. In a study for the RECORD organization, on methods for estimating and optimizing the quantities of contaminated land to be treated (Jeannée and Demougeot-Renard, 2016), a questionnaire was sent to professionals of contaminated land remediation, to collect feedback regarding discrepancies observed between estimates resulting from the investigation phase and the remediation phase. The results of this questionnaire illustrate how the uncertainties associated with the investigation, analyses, or interpretation phases can strongly influence the objectives of the remediation works and lead to financial (or even liability) risks for companies.

Among the practical answers to this questionnaire, it was noted in particular that commonly-used analysis packs (standard series of analyses) are often insufficient to reliably validate the choice of remediation techniques, that the diagnoses are often too inaccurate in terms of the thickness of the contamination, that there is often a lack of information on, e.g., the presence of water in the boreholes, or of volatile compounds, etc. Here too, the use of clean-up targets other than "yes-no thresholds" (see section 2.4.7) might help to better manage uncertainties.

2.7. Data/metadata storage

Data storage is an essential aspect of managing contaminated land, for informing stakeholders about the risks associated with these sites and for maintaining a memory of the sites in relation with possible usage constraints. At the request of the French ministry, the BRGM conducts a census and disseminates information regarding former industrial activities in France. The administration is also responsible for monitoring and communicating on contaminated (or potentially contaminated) land requiring preventive or curative action by public authorities. These are the BASIAS and BASOL databases, resp., which are available to the public. Of the 318,000 BASIAS sites that have been industrially active in the past, approximately 7,000 are subject to specific monitoring and are referenced in BASOL.

More recently, the BRGM, with the support of ADEME, is currently developing the BDSolU database, which contains chemical analyses of soils taken from urban areas, as well as information regarding sampling conditions, etc. These data improve knowledge of the geochemical quality of urban soils and the definition of anthropized pedogeochemical backgrounds. The dedicated website allows the online storage of soil analyses generated by declared suppliers of information and the consultation of data made available to the public. The issue of uncertainty is addressed in the BDSolU database, with a specific field for laboratories to provide information on analytical uncertainties (section 2.3). Other sources of uncertainty, regarding, e.g., sampling point x and y coordinates, could also be addressed.

Key issues in data storage and stakeholder dissemination include the establishment of links between different bases, which relates to data interoperability (their use for different applications or platforms that can communicate with each other). One area of interoperability that is currently under discussion in the field of contaminated land management is BIM (Building Information Modeling; see Molleron, 2019), which allows in particular a 3(4)D visualization of data throughout the life cycle of a building, infrastructure, etc. Among the research and development challenges there lies the question of how BIM can communicate with soil quality databases.

3. Further research

3.1. Introduction

This brief and very partial overview of the notion of uncertainty in the data cycle associated with contaminated land management illustrates the variety of issues that are relevant for a decision-support process that is efficient and consistent with available information. Uncertainties are inherent in any environmental study and no methodology will help eliminate them entirety. Certain types of uncertainty simply cannot be quantified, since we cannot quantify what we do not know at all: it can be issues that are poorly understood from a scientific viewpoint, such as the synergistic toxicity effects of contaminant mixtures, or the behaviour and effects of certain emerging pollutants, etc.

But we can at least try to reduce uncertainties by implementing appropriate techniques (of sampling, analysis, etc.) and try to take them into account in a coherent way to inform the decision-support process. The following sections present some lines of research, again with reference to the diagram of **Figure 1**.

3.2. Sampling

With respect to sampling environmental media (soil, water, gas, etc.), further work is needed to improve the representativeness of sampling and analyses, on the one hand by optimizing sampling strategies as a function of knowledge regarding pollutant behaviour and their spatial distribution considering historical and documentary studies and, on the other hand, by improving field methods that prevent the physical-chemical evolution of samples during their transport to the laboratory.

The development of indirect methods (geophysics, etc.) is to be pursued in order to optimize the localization of sampling points. The approaches developed in recent years to characterize *in situ* contaminant fluxes, rather than just concentrations, should be developed to help focus treatment methods on areas which contribute the most to contamination and generated the most risk for groundwater resources for example.

3.3. Uncertainty related to laboratory analyses

For this aspect, among the options offering prospects for future work, one may include:

- a synthesis of data on "the profession's estimation" of uncertainties regarding key parameters for matrices of interest in contaminated land management;
- the implementation of inter-laboratory testing for "orphan" parameters (for which there are currently no tests on the market) and the preparation of reference materials for key parameters. The aim would be to verify the accuracy and comparability of results for these parameters;
- to estimate the relative uncertainties associated with the physical preparation of the samples in the laboratory (quartering, grinding, etc.) versus the analysis step.

3.4. Representation and use of uncertain information

3.4.1. Representation of uncertain information

As suggested above, the chart in **Figure 18** needs to be clarified in order to better identify the conditions of application of the various mathematical tools for representing and propagating uncertain information. But beyond this chart, further work could address the issue of expert judgment representation, which is an essential source of information in the practice of contaminated land management. It would seem appropriate to carry out this study in relation to the various databases developed over the years in this context (on soils; BASIAS, BASOL, ASPITET, DONESOL, BDSolU, on plants; BAPPET, BAPPOP, on air quality, etc.), since expert judgment draws a lot from such sources of information.

3.4.2. Imprecise thresholds

Section 2.4.6 illustrated the idea of an imprecise threshold (or fuzzy threshold). This concept could be "tested" in real cases of contaminated land management. First, in terms of their construction (gathering information, interpreting and representing imprecise risk thresholds). And secondly in terms of communication with stakeholders (section 2.5) for various field situations.

3.4.3. Constraint-limited compliance with a threshold

A common objective in contaminated land management, is to define a soil quality concentration such that the estimated risk from a “model” remains below an acceptable risk threshold (e.g. the 10^{-5} threshold for individual excess risk in the case of known carcinogens). The inverse problem consists in estimating this quality in an automated way, taking into account constraints associated with the factors that influence risk. If some of these factors are incompletely/imprecisely known and represented using possibility distributions, we are faced with a problem of optimization under fuzzy constraints. While there are several examples in the literature regarding the application of this type of approach, to our knowledge it hasn’t yet been applied to the context of contaminated land management.

3.4.4. Geostatistical methods

a) Continue to improve the estimation of highly contrasted soil concentrations

Previous work has already highlighted the usefulness of "discrete disjunctive kriging" for estimating highly contrasted concentrations. Developed for the mono-variable case, this estimator must be adapted to the multi-variable case: several substances; co-variables such as soil composition or fast on-site measurements, etc.

Further tests need to be carried out, for different organic or metal contaminants. A guidance document could help make this method more easily applicable by consulting companies, taking into account the specific aspects of soil contamination, such as the often-observed vertical non-stationarity of concentrations.

Finally, model comparisons (top-cut approaches, disjunctive kriging with different spatial distribution models) should be performed for different types of contaminants (metallic, organic). The results would be useful in view of their implementation by consulting companies.

b) How to define the anthropized pedogeochemical background?

Estimating the anthropized pedogeochemical background from a decomposition of concentrations following different scales of variability provides a precise meaning to the geochemical background. But several questions remain:

- How to go from a map to a "soil concentration threshold" for the purpose of excavated soil management?
- What value should be given to the background threshold: a spatial average, a local maximum or a quantile on a mesh? What should be the support?
- Compare the current method of decomposition by kriging analysis (based on the different spatial structures highlighted by the concentration variogram) with a decomposition based on classes of soil concentration (by discretizing the concentration) in order to better characterize levels of "anomalies".

Indeed, in the estimation of the "background" by factorial kriging, the average of the anomalies is zero (Sauvaget, 2019). This property is interesting as the soil concentration may be lower than the estimated geochemical background, which is useful for the management of excavated soil. But there are other methods of decomposition of the concentration into components, associated with different spatial variability

"scales", such as the one implemented in the KDD (discrete disjunctive kriging) model. In this model, the concentration can be seen as an addition of successive values (intervals from 0 to 10 ppm, 10 to 50 ppm, 50 to 150 ppm) weighted by the indicators (known and equal to 0 or 1), each class indicator having its own variogram.

This could provide a more “detailed” description of the spatial variability of soil concentrations by intervals of values rather than the decomposition by factorial kriging and which might “solve” the question of the component average (zero for the “anomalies” from kriging analysis). The comparison of these two decompositions of the concentration by variability scale (kriging analysis and KDD) might help clarify the “physical” meaning of the pedogeochemical background, by specifying how successive “value intervals” contribute to the spatial variability. Schematically, where factorial kriging takes only into account scales of spatial variability, the proposed disjunctive kriging approach simultaneously considers the value classes (low, intermediate or high) each with their own spatial variability. Also, the multivariate modelling should be considered, as for kriging analysis.

In the case of data with a significant heterogeneity of distribution (numerous in some areas but scarce in others, with clustering effects), the combination of methods by kriging and using fuzzy estimators would also deserve to be explored. Such a research axis would be an opportunity to revisit the work of Loquin and Dubois (2012) on kriging with imprecise data and variograms. One might also examine the potential contributions of AI (artificial intelligence) in this context: by exploiting considerable amounts of data, could AI help to identify correlations that better highlight anomalies and, by difference, what can be considered as the pedogeochemical background (in a "non-anomaly" sense)?

3.5. Communication with stakeholders

While the use of imprecise thresholds (with a transition zone) may have methodological benefits, there remains the question of how they might be received in a context of communication with stakeholders. There is on the one hand, the potentially exposed populations, and also the regulatory officers who must make decisions regarding management measures. In this context, it is necessary to include input from the social sciences in order to develop methods and tools to help build a shared understanding of issues related to contaminated land management and associated uncertainties. This applies, for example, to constraints associated with the use of contaminated land (e.g., a ban on the consumption of self-produced vegetables, or on the consumption of water from private wells, etc.). If such constraints are not first understood by local populations, they cannot be accepted or implemented.

"Serious games" or participatory simulation approaches are beginning to be increasingly used to engage with stakeholders and to better integrate collective intelligence into the management of degraded sites. This is the case, for example, for water use conflicts (Barnaud et al., 2007). Participatory simulation combines modelling with participatory approaches to promote social learning regarding environmental issues (Becu et al., 2017). Multi-actor role-playing (collective situation simulation and social learning) addresses questions such as: what type of individual or collective decisions, of which actors, have which influences on contaminated land management (or its equivalent in the game)? Such tools can help identify the diversity of judgments and perceptions of the various actors, in relation to their own experience of contaminated land management.

3.6. Use for management and monitoring

Among the advantages of representing partial ignorance when propagating uncertainties are the possible consequences in terms of management and monitoring: if the difference between the lower and upper bounds of the probability of complying with risk objectives is too large, the study might enter a new acquisition phase in order to reduce uncertainty. This approach would typically involve a sensitivity analysis to identify which parameters should be investigated in priority in order to reduce overall uncertainty. A cost-benefit approach could also be performed in this context.

An essential step in contaminated land management is the termination of clean-up operations (when, how, according to which criteria?...). Taking into account uncertainties in the definition of criteria for stopping such operations would seem very relevant.

But following all the investigations and the implementation of remediation operations, it is possible that incompressible uncertainties remain regarding environmental quality acceptability and/or health risks. In this case, compensatory measures can be considered, such as construction mitigation measures (e.g., air vacuum systems for the prevention of soil-vapour intrusion).

3.7. Data and metadata storage

Information about uncertainties associated with the various stages of the acquisition of environmental data is often lacking in databases. While an obvious reasons for this is the relative complexity of the problem, it is likely that the often-assumed obligation to apply a conventional probabilistic framework may also hinder progress on this issue. Indeed, the application of this framework assumes that the uncertainty at each stage of the acquisition can be characterized (in the Gaussian case) by a standard deviation around an average value and that the interactions between the stages are sufficiently well known (and quantifiable) to derive an overall probabilistic uncertainty. Faced with the difficulty of such a task, the tendency is either to ignore the question of uncertainties altogether (the most frequent option), or else to provide a very partial indication (for example, by focusing solely on analytical uncertainty, since this the topic of existing standards; see section 2.3).

Yet other approaches could be explored. In particular, in relation with a “rehabilitation” of the notion of interval in environmental monitoring, the field investigator (who is the person most apt to describe the uncertainty relative to his/her measurement), could provide an interval on the basis of an expert judgment, the extent of which would depend on sampling conditions (good versus bad). Thus, in the database, a measure would not be represented by a single value, but by an interval with one or more preferences provided for that interval. Alternatively, the quality of the measurement could be qualified by an indicator of reliability (e.g., a number between 1; not reliable and 5; very reliable).

The issue of the uncertainty representation for data stored in databases raises the question of the interoperability of these databases with other tools. One may think, for example, of establishing links between BIM (Building Information Modelling), which is increasingly developed to manage and represent data on buildings and infrastructures throughout their life cycle, and information on soil quality in a context of brownfield development for example. While work on the interoperability between different databases is currently under way (e.g. mind the MINDD project; http://www.minnd.fr/), the issue of data uncertainty representation in these databases is certainly worth exploring.

4. Conclusions

As stated in the introduction, this document has no claim to completeness and only scratches the surface of the issue of managing uncertainties in a context of contaminated land management. It nevertheless helps to clarify some fundamental questions, such as: what is the difference between knowing and not knowing in this context? The answer to this question has direct consequences on the choice of methods for representing and propagating uncertainties in, e.g., risk assessment tools and several examples of such methods are presented in this report.

This question seems especially relevant at a time when the myth of the "omniscient expert" is clearly a thing of the past. Indeed, the societal reality of contaminated land management today (or more generally "degraded" sites such as, e.g., former mining sites) is typically one where the "official expertise" is questioned, with the emergence of an alternative expertise (which in many cases may prove very relevant; hence the utility of developing a collective intelligence in this context). Given the complexity of the mechanisms influencing contaminated land, the expert certainly has the right not to know (everything) and it is therefore recommended that lack of knowledge should be documented. Indeed, the display of certainty in spite of real uncertainties, in a context of “aversion to risk” (as is the case for contaminated land), can be counterproductive since facts can rapidly contradict the apparent confidence (facts are often stubborn ...).

In this type of situation, the "distrust" mentioned previously regarding the official expertise may lead to a search for liabilities. Yet a better consideration of uncertainties, particularly of an epistemic nature (related to incomplete knowledge), combined with a more shared understanding with stakeholders of the various issues related to contaminated land management, might help improve confidence between the various actors of this field.

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INDEX OF TABLES AND FIGURES

FIGURES

ACRONYMS

ADEME	French Environment and Energy Management Agency
BRGM	French Geological Survey
IRIT	Toulouse Research Institute in Computer Science
Mines ParisTech	Paris School of Mines

ADEME IN BRIEF

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EXPERTISES

TAKING INTO ACCOUNT UNCERTAINTIES IN CONTAMINATED LAND MANAGEMENT

Abstract This document is a synthesis on uncertainties in the field of contaminated land management. The synthesis, which has no claim to completeness considering the scope of the problem, focuses on identifying sources of uncertainty at different stages of the data cycle in a context of contaminated land management, on describing approaches that are proposed to address these uncertainties and on avenues for further research.

The considered data cycle ranges from the environmental media sampling stage, to the use of the collected information for defining management choices, through analysis, representation, interpretation, etc.

This synthesis illustrates in particular that while there exists no "one-size-fits-all" method for addressing uncertainties in a context of contaminated land management, it is nevertheless possible to promote consistency between the choice of methods for addressing uncertainties and the nature of the information that is actually available. This search for consistency is expected to foster more reliable and robust management choices.

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