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Initial nuclear state characterization in view of decommissioning: STRATEGIST, a data analysis & sampling design web tool

S. Boden[1*], B. Rogiers [1], Y. Desnoyers[2], N. Pérot[3], G. von Oertzen[4], O. Sevbo[5], S. Demeyer[6]

[1]SCK CEN, Belgian Nuclear Research Centre, Boeretang 200, B-2400 Mol, Belgium
[2]Geovariances, 49bis avenue Franklin Roosevelt, 77210 Avon, France
[3]CEA, DES, IRESNE, DER, SESI Cadarache, 13108 Saint Paul-Lez-Durance, France
[4]Brenk Systemplanung GmbH, Heider-Hof-Weg 23, Aachen, Germany
[5]Energorisk, Simyi Steshenkiv str. 7, Kyiv-03148, Ukraine
[6]LNE, 29 avenue Roger Hennequin, 78197 Trappes Cedex, France
[*] Corresponding Author, sven.boden@sckcen.be

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Abstract

The INSIDER project (2017-2021, (LGI, 2017)) developed and validated a new and improved integrated characterisation methodology and strategy during nuclear decommissioning and dismantling operations (D&D) of nuclear power plants, post-accidental land remediation or nuclear facilities under constrained environments. One of the important outcomes of this strategy development is a statistical approach guideline, that is transformed into a web tool, which serves as a more user-friendly interactive interface. The web tool, named STRATEGIST (Sampling Toolbox for Radiological Assessment To Enable Geo-statistical and statistical Implementation with a Smart Tactic), intends to guide the expert in handling the problem definition and applying a strategy based on proper data analysis and sampling design. It is not meant to provide the nonspecialist with a comprehensive mode of operation for the complete process of initial nuclear state characterisation in view of decommissioning.

This paper describes the approach followed to **develop** the guideline and **STRATEGIST web tool**, based on state-of-the art statistical techniques for preliminary analysis and data processing. Furthermore, it briefly outlines the web tool contents and structure. The initial guidance was adjusted and finalized, based on its implementation into four different use cases, which are concisely summarized as well. **Lessons learnt** from this implementation are listed in terms of overall strategy implementation, selection of sampling approaches and data analysis methods and are complemented with a specific focus on uncertainties. They illustrate that the implementation of a proper data analysis and sampling design strategy simplifies and optimizes the decision making process concerning the selection of the different D&D scenario options.

Introduction

Decommissioning and dismantling of all types of nuclear facilities until their remediation and clearance, is a global international industrial challenge of the 21st century. Nuclear waste from decommissioning occurs in a wide variety of matrices and contaminants. Proper radiological and chemical characterisation of plant areas are a necessary precondition for a successful project regarding the definition of viable dismantling scenarios and the classification and segregation of the different impacted (e.g. contaminated, activated) materials. As such, initial characterisation is an essential part of the decommissioning cost estimation process. It is essential to act on the upstream stage of the dismantling for the management of all radioactive waste. Lessons learned on past decommissioning projects reported the importance of a suitable sampling strategy to detect and treat accumulated contamination and of a complete qualitative and quantitative characterisation at early stage for fissile material monitoring. The lack of knowledge and accessibility constraints within nuclear facilities complicates the mapping and cartography of the radiation levels. In some cases, this leads to partial in-situ mapping and off-line analysis of biased samples, finally causing extra technical and budgeting problems. In this respect, "statistical modelling to optimise sampling" was one of the challenges identified by the Nuclear Energy Agency Working Party on Decommissioning and Dismantling (WPDD) in its report on R&D and innovation needs for decommissioning of nuclear facilities (WPDD-NEA-OECD, 2015).

The INSIDER project, initiated in 2017, aims at developing and validating an improved integrated methodology of characterisation based on a state-of-the-art statistical processing and modelling techniques,

coupled with present (and adapted) analytical and measurement methods, with respect to sustainability and economic objectives. One of the important outcomes of this EU horizon 2020 project is the STRATEGIST web tool for guiding the application of such a statistical approach.
This paper describes the approach followed to develop a guideline, which was further transformed into a web tool, by experts of the following organisations: Brenk Systemplanung, CEA, Energorisk, Geovariances, LNE and SCK CEN (in alphabetical order). We only briefly describe its contents considering that the tool is directly available on the internet (INSIDER, 2019). The aim of the statistical approach guideline is not to provide the nonspecialist with a comprehensive mode of operation for the complete process of initial nuclear state characterisation in view of decommissioning. Nor is the proposed approach pursuing to be a stepping-stone towards international standardization. This is amongst others due to the complexity of the full process, where in some cases massive data coming from various sources (on-site and lab measurements, destructive and non-destructive measurements) are being generated, while in other cases only very limited data is available. Moreover, the scope could cover all levels of activity concentrations, type of radionuclide compositions and volumes and masses of material types originating from nuclear installations, buildings and sites. Accordingly, the web tool merely intends to guide the expert in handling the problem definition and applying a strategy outlined in the STRATEGIST web tool. It is only a guideline, and should not be followed blindly. Special circumstances often ask for special solutions, which cannot be covered exhaustively by a generic strategy. This strategy can be used to inform people with no or very little experience in statistics about the complexity of the issue, and provide them with some relevant background, but it cannot justify not involving people experienced in the matter.

Development of the STRATEGIST web tool

Initially, we compiled an overview of sampling design methods described in standards and guides, followed by a brief presentation of the statistical methods available that can be used to demonstrate meeting the objectives in the context of initial nuclear site characterization in constraint environments. This resulted in a report on the state-of-the art (Pérot, et al., 2019), available on the INSIDER project website (LGI, 2017). Consequently, the statistical methods were organized in such a way that the end user is guided towards the appropriate statistical methods (including, but not limited to those identified in the state-of-the art report) for data analysis and sampling design ((Rogiers, et al., 2018), (Desnoyers & Rogiers, 2018) and (Desnoyers & Rogiers, 2020)). To aid the end user in applying this strategy, the user-friendly web application STRATEGIST was made freely available (INSIDER, 2019). Its contents and functionality are briefly described in the next section in this paper. The validation phase then consisted of implementing the strategy in four different so-called “use cases”, covering studies on decommissioning projects of a nuclear research facility, a nuclear power reactor and a post-accidental site remediation. This paper gives a very brief description of the use cases and provides an overview of the lessons learnt. Assessment of the return of experience resulted in a refinement of the statistical approach guideline and tool.

Contents and structure of the statistical approach guideline & tool

For detailed information, we refer to the STRATEGIST web tool (INSIDER, 2019). The tool is structured using a sequence of descriptive diagrams. The **overall strategy diagram** (Figure 1) outlines the general steps between a request for initial characterization and reporting of the final results, after all objectives have been reached. The different steps related to the actual data analysis and sampling design are strongly dependent on the situation, the available data and the specific goals and constraints. This is represented in the diagram in Figure 2. The exploratory **data analysis** has been structured in a way that it is applicable to most problems in D&D for constrained environments, by looking into four aspects of the data:

- Is this a univariate or multivariate problem?
- Is this a problem involving spatial trends?
- Is this a problem involving spatial structure?
- Is this data requiring robust methods?

This only provides some guidance on the type of methods to use, and the expertise of the user of this strategy comes in at this point to make a final decision, based on the individual method descriptions, suggestions and remarks contained in the tool. The **list of methods for data analysis** are organized in a Venn diagram (Figure 3) according to the four aspects of the data mentioned above. All methods mentioned on the Venn diagram are discussed separately or as part of a broader type of methods, in which case they are mentioned in the text. Clicking on the method will give the user a concise description of the method. In order to help the end user to get started, the tool provides a list of theoretical examples, software implementations, example use cases and references. Similar to the data analysis, the STRAT-EGIST web tool provides general **recommendations for the sampling design approach**, making a distinction between probabilistic and non-probabilistic approaches, and designs with equal or non-equal probability of selection (Figure 4).

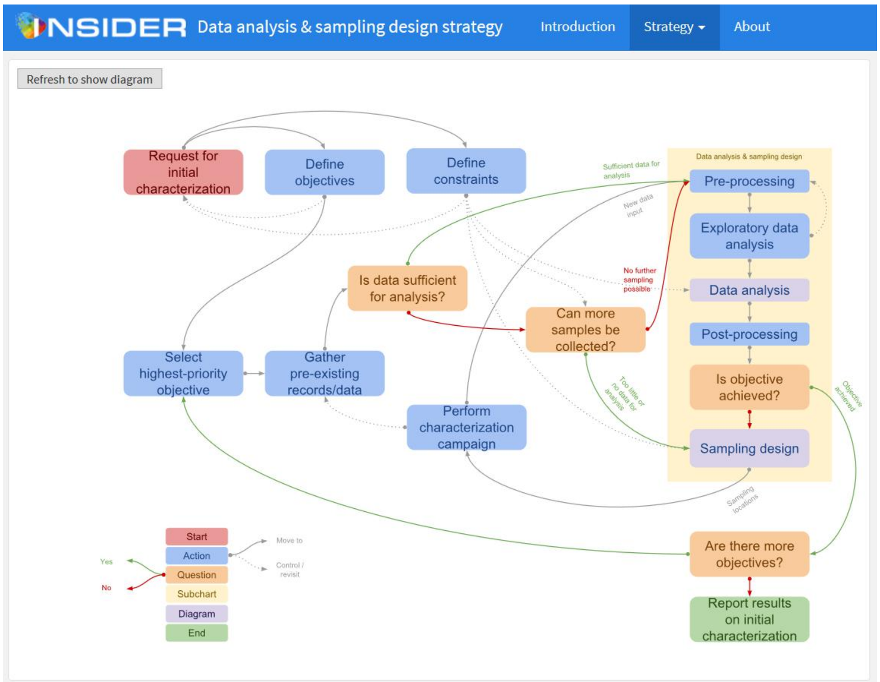

Figure 1: STRATEGIST: overall strategy diagram

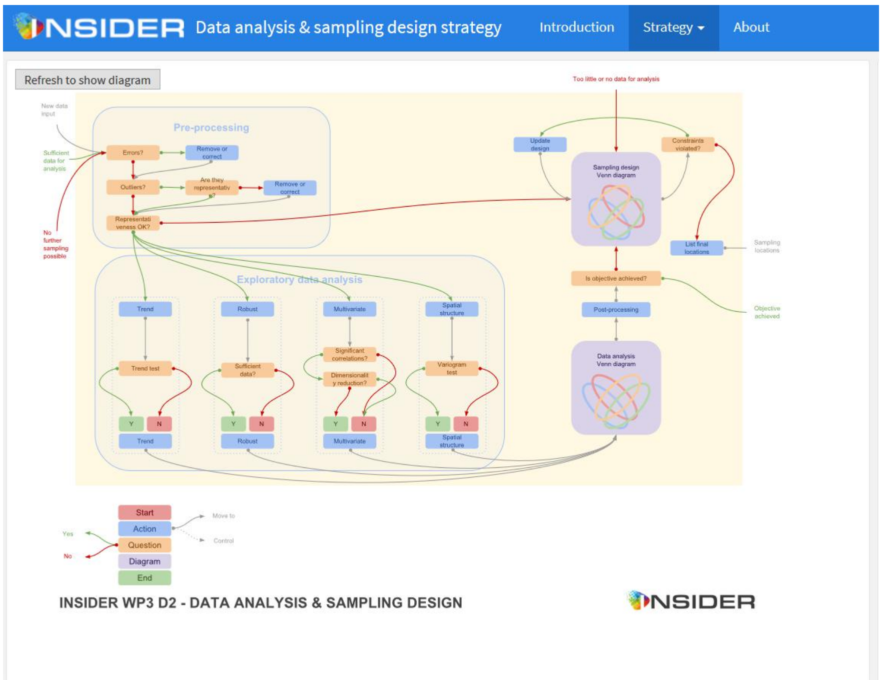

Figure 2: STRATEGIST: data analysis & sampling design diagram

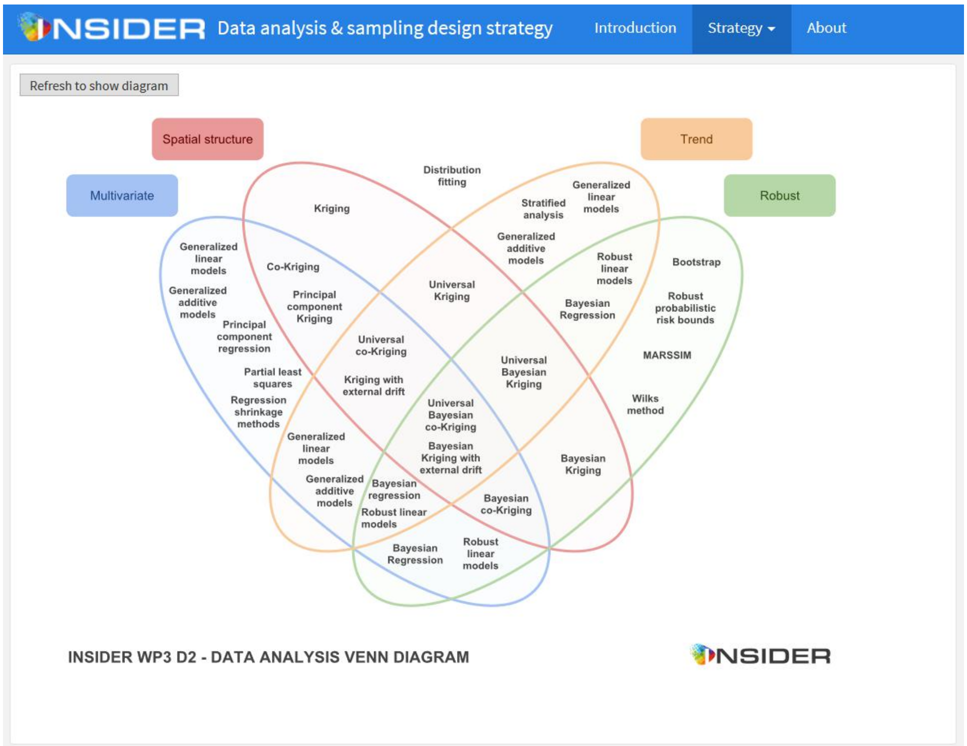

Figure 3: STRATEGIST Venn diagram listing the methods for data analysis by looking into four aspects of the data: univariate or multivariate, spatial trends, spatial structure and robust methods. All methods mentioned on the Venn diagram are discussed separately or as part of a broader type of methods, in which case they are mentioned in the text. Clicking on the method will give the user detailed information on the workflow, example of software implementations, example use cases and references.

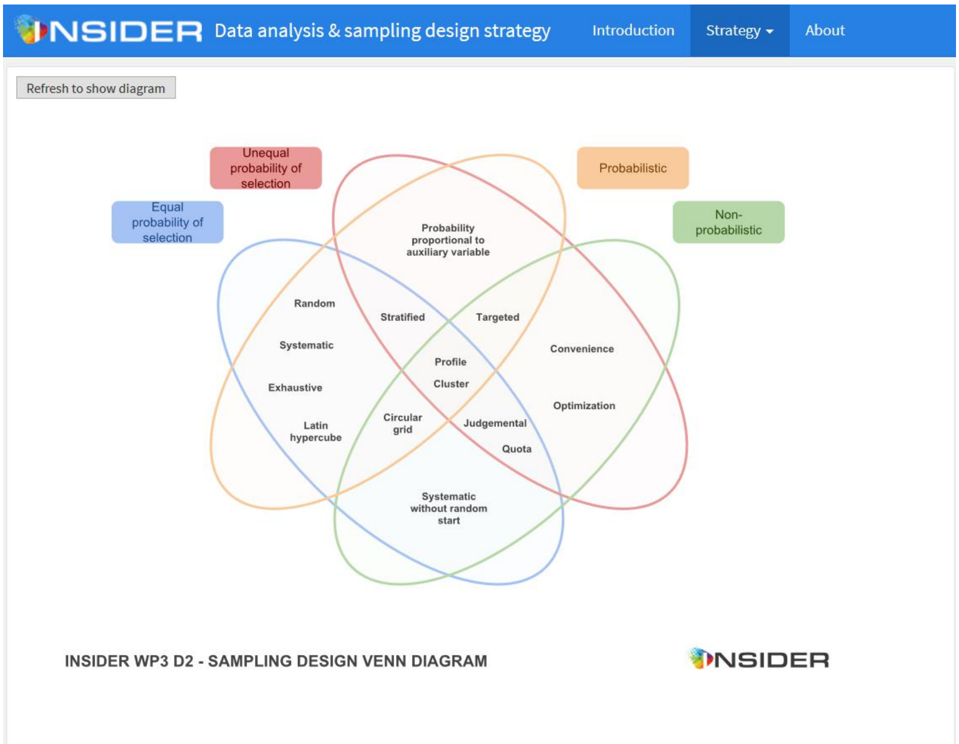

Figure 4: STRATEGIST Venn diagram showing a non-limitative list of sampling design approaches organised according to the following questions: probabilistic or not and selection probability equal or not.

Implementation in four use cases
The statistical approach presented in the STRATEGIST web tool was implemented in four different use cases:

- **UC1**, concerns two tanks (VA001 and VA002), each about 50 m³ in volume, **containing low level liquid waste (LLLW)** and located in the liquid waste storage facility at the Joint Research Centre site of Ispra, Italy. The specific activities of the radionuclides present are between a few tenths to just over 100 Bq/g (2012-2013) for relevant nuclides, which include gamma emitters Co-60, Cs-137 and Am-241 as well as various alpha-and beta emitters (von Oertzen, et al., 2020). The licensee had not specified any waste acceptance criteria for this waste. Moreover, no information was available on what the conditioning process prior to waste acceptance should be. Within the INSIDER project, we therefore defined the following artificial objective: characterize the radionuclide content of the tanks, in view of deciding if the waste acceptance criteria for the selected waste category could be met. As a basis, we used the waste acceptance criteria for the Konrad repository (Germany).
- **UC2** involves the **biological shield** of the Belgian Reactor 3 (BR3), a pilot pressurized water reactor of the SCK CEN (Belgian Nuclear Research Centre). The reinforced concrete shielding represents a volume of about 622 m³ (> 2000 tons). The concrete close to the reactor pressure vessel is activated. The main goal was to develop a radiological characterization program aiming at economically optimizing the biological shield dismantling strategy using a waste-led approach (Broeckx, et al., 2020).
- **UC3a** relates to a nuclear facility that was devoted to radiochemistry on trans-uranium elements. It was under operation until 1992 on a CEA site in France. Due to different incidents decades ago, the **soil beneath** the **tank room** is contaminated with various alpha and beta emitters up to several TBq. For the preparation and management of a soil remediation project, some global quantities such as the average activity concentrations and total activity for the whole area (as well as its related uncertainty and confidence level) need to be estimated in a sound way (Desnoyers, et al., 2020).
- **UC3b** covers the **graphite** moderator and reflector (about 1300 tons) of the G2 UNGG reactor localized at the CEA site of Marcoule. The main objective is to provide a radiological inventory for the graphite volume. Some specific nuclides will be of key interest from a waste disposal perspective. A secondary objective is waste oriented with the classification of volumes according to different thresholds.

Detailed reports of the implementation and findings are described in separate annexes to the guidance document and will be available in the STRATEGIST web tool. This section only summarizes the use cases key parameters. Annex 1 of this paper summarizes the main properties of the four use cases and the selection of sampling design and data analysis methods. The four cases represent four different materials: an aqueous solution containing a limited amount of sludge, high density concrete including metal reinforcement, soil and graphite. Two cases are related to neutron induced activation (UC2 & UC3a) and the other two cases (UC1 & UC3b) are more closely related to contamination. The maximum activity concentration levels are expected to be in the range of 100 Bq/g for UC1, UC2 and UC3a, but will be higher for UC3b. In all cases, the objective is somehow related to compliance with (waste) acceptance criteria and/or a categorization (e.g. exceeding a threshold). The volumes considered in the scope are generally large (100-600 m³). The size of the final dataset available is strongly dependent on the case. The number of available data points increases from UC1 and UC3a up to UC3a and UC2. Unfortunately, it was not possible to test the full implementation in all use cases, due to practical constraints. UC3a and UC3b were limited desktop exercises, where data analysis was performed on existing data sets without having an impact on the sampling design strategy. The reporting in annex 1 regarding sampling design for UC1, UC3a and UC3b is valid for the prior data and should not be considered as the sampling design strategy selected according the STRATEGIST web tool. In the case of UC1, some additional samples were taken during the INSIDER project. However, also in this case there was no impact on the sampling design due to sampling constraints for the tanks. The additional results from the supplementary sampling and INSIDER in-situ measurements have not been taken into account in the data analysis process. They only have been used for quality control purposes. Eventually, the only case that followed all steps of the STRATEGIST overall strategy diagram was UC2. Figure 5 shows the overall strategy implementation for UC2, consisting of three stages:

- Stage 1, starting with the request for initial characterization, performing a preliminary data analysis based on pre-existing data and followed by sampling design since this was not sufficient to achieve the objectives (dotted arrows).
- Stage 2, starting with the performance of a characterization campaign, followed by a second data analysis of the increased data set and completed with a sampling design since the initial objects were still not fully achieved (dashed arrows).
- Stage 3, gathering the additional data followed by a third and final data analysis of the full data set. The data and model were considered adequate for meeting the objectives (solid arrows).

We further point out that for most use cases various methods for data analysis have been selected and implemented.

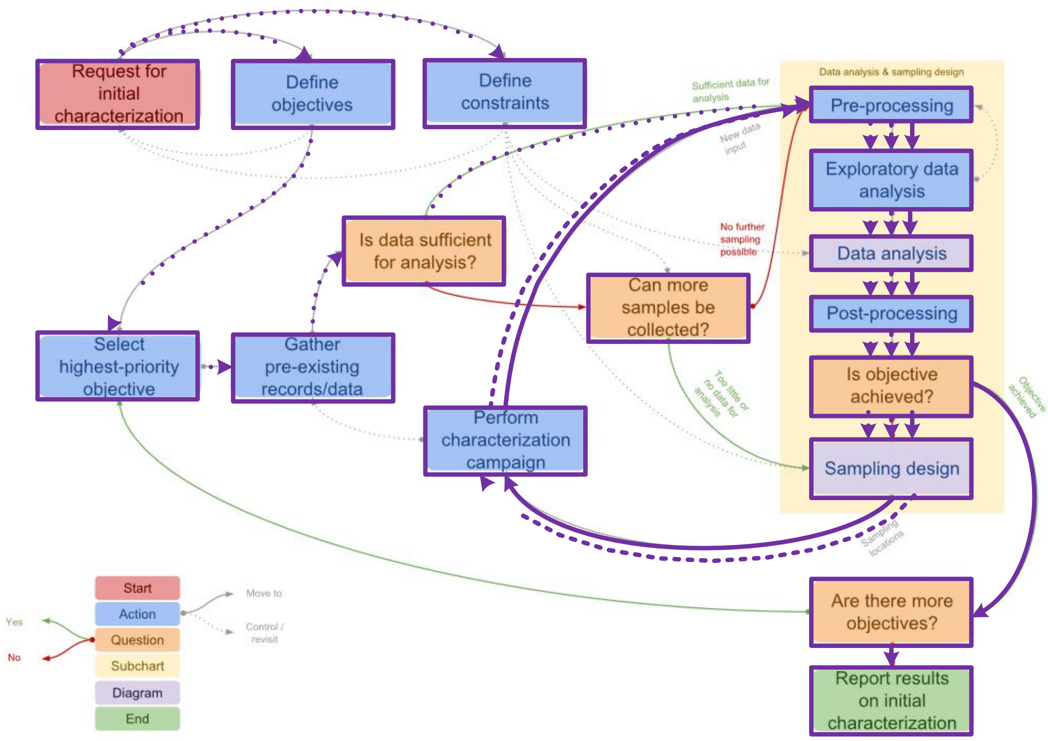

Figure 5: Visual representation of the overall strategy implementation in three stages for UC2. The purple arrows show the process flow in each stage: stage 1 (dotted arrows), stage 2 (dashed arrows) and stage 3 (solid arrow).

Lessons learnt

Lessons learnt are summarized below according to the structure of the STRATEGIST web tool: general aspects related to the overall strategy and specific elements related to the sampling design approach and the data analysis methods. We conclude with a specific discussion dedicated to uncertainties.

Overall strategy

Very clear and quantifiable **objectives** allow the development of an effective sampling plan, including the selection of appropriate measurement techniques and the up-front definition of criteria for the measurements (e.g. detection limits, uncertainties). On the contrary, the absence of explicit objectives complicates all aspects of designing and implementing the characterization strategy and the planning down to the selection of appropriate measurement techniques, determination of minimal detection limits, etc. This is illustrated in UC1. If feasible, data sets containing large amounts of below **detection limit** data

should be avoided and whenever possible tackled during the strategy development (e.g. UC2). However, this is not always possible; for example due to low threshold values, the limitations of measurement techniques, but also due to unclear initial objectives or potentially changing objectives or thresholds during the characterisation process. Depending on the case, it might be very wise to use advanced statistical methods for dealing with samples below detection limit (Kim, et al., 2020). In UC1 and UC3a, data analysis methods were tested with and without uncertainties and data below detection limit were applied. Especially UC3a shows that the impact on certain parameter estimates can be significant.
Performing a radiological characterization program in two or more **stages/phases** as implemented in UC2 can be efficient and effective to tackle areas with higher uncertainties. Unfortunately, this might not always possible due to planning constraints. In addition, historical data, sometimes gathered with other objectives (e.g. analysis liner samples in UC2) could optimize the characterization process.
In a first attempt to organize and select methods for sampling design and data analysis, we produced streamlined flowcharts including yes/no answer questions and decision trees. However, this approach was abandoned rather soon and replaced by the organization of a non-limited list of methods in Venn diagrams, guiding the end-user to the selection of appropriate methods. Indeed, there is not a unique and absolute solution. This **flexibility for the selection of suitable methods** is vital, since the same problem can be tackled using various methods as mainly demonstrated in UC1, UC3a and UC3b.
Figure 6 and Figure 7 represent the various sampling design approaches and data analysis methods used. In UC1 for example, the mean value of the activity for several nuclides was calculated using various robust methods. The methods included empirical mean, Wilks median, bootstrap estimation of mean, Bayesian estimation and mean estimated from a fitted theoretical distribution law. The Wilks method provided the most conservative estimates, particularly so for data sets with outliers.
Decommissioning is a multi-disciplinary operation and the **involvement** of specialized staff performing the next stages of the decommissioning project has proved to be beneficial in UC2. Technical feasibilities/constraints in the next stages might strongly influence the initial characterization program. Effective communication and common understanding is essential. Extensive compartmentalizing might result in misinterpretation and wrong decisions.

Sampling design approach

In case of tanks filled with liquids as in UC1, there is always an amount of sludge present. **Representative sampling** is obviously a challenge in this case. In theory, one should sample the population as a fully homogeneous entity. According to the historical information, this might have been more or less the case for the historical sampling campaign of UC1. An alternative is to apply stratified or targeted sampling of solid and liquid fraction after settling. The latter was however not feasible due to accessibility constraints. Instead, additional samples were taken during the INSIDER project after trying to homogenize the contents of the tanks for a few hours. Results from sample analysis showed a large level of heterogeneity, resulting in the cancellation of the INSIDER benchmarking exercise.
As shown in Figure 6, the sampling design approach is not uniquely defined in all of the real use cases. Often, a combination of approaches is being implemented. In any case, the **sample locations** should be selected so that subsequent extrapolation during data analysis is avoided. As shown in UC2 (stage 2) and UC3a, this does not only concern the expected activity concentrations (lowest and highest), but also the physical location. It is obvious that in a certain stage in the dismantling process, it might be difficult or impossible to access locations with expected extreme values for performing in-situ measurements or for taking samples. In this case, it is necessary to foresee the measurements at a later stage in the project and to allow for updating the existing data analysis and post processing. Just ignoring the information might result in unacceptable uncertainties. Many characterisation projects have the tendency to focus their sampling efforts on the highest affected areas, neglecting areas with lower activity concentration levels. Nonetheless, it is necessary to sample the supposedly least impacted zones as well as the most impacted zones to achieve a realistic understanding of the statistical distribution of the activity concentration. Confirming some non-impacted areas is often as important as (or even more important than) confirming historically impacted areas. From the point of view of waste volume management, transition zones are more critical, since it is difficult to categorize them with respect to the reference thresholds. Uncertainty being the most important in these areas for proper delineation (and limiting misclassification errors), the sampling distribution should favour them over other areas that only require confirmation of impacted or non-impacted.

Defining the **sample size** or density often results in lively discussions, due to the impact on planning and overall costs. The STRATEGIST web tool provides for example a computation of the minimal sample size to estimate a quantile (or a tolerance interval) with a given confidence level according to Wilks formula. However, implementing it in day-to-day practice might be challenging when several physical parameters need to be assessed (i.e. total activity, activity concentration, thresholds) based on various data sources that might not always be representative. Moreover, a data set might contain considerable amounts of values below detection limit and confidence levels required might not always be unequivocally defined. Sensitivity analysis on the UC2 data showed that reducing the size of the primary dataset with about 75%, could result in extreme under/over estimation of the volume exceeding the threshold. The sensitivity analysis also shows that this deviation can be strongly reduced by combining the limited higher quality and costly primary dataset (in-lab sample measurements) with a large cheap secondary data set (in-situ measurements). Also in the UC3a case the effect of sample reduction was examined. Due to the already limited amount of cores, the total number of samples was decreased by reducing the number of samples in each core in a systematic way, attempting to keep spatial sample distribution. Sample reduction generally leads to an increasing uncertainty and estimated remediation volume. The effect is still limited for a 50% sample reduction but can strongly increase when sample density is further reduced. Also in this case, the additional uncertainty can be mitigated by integrating secondary data from gamma scanning.

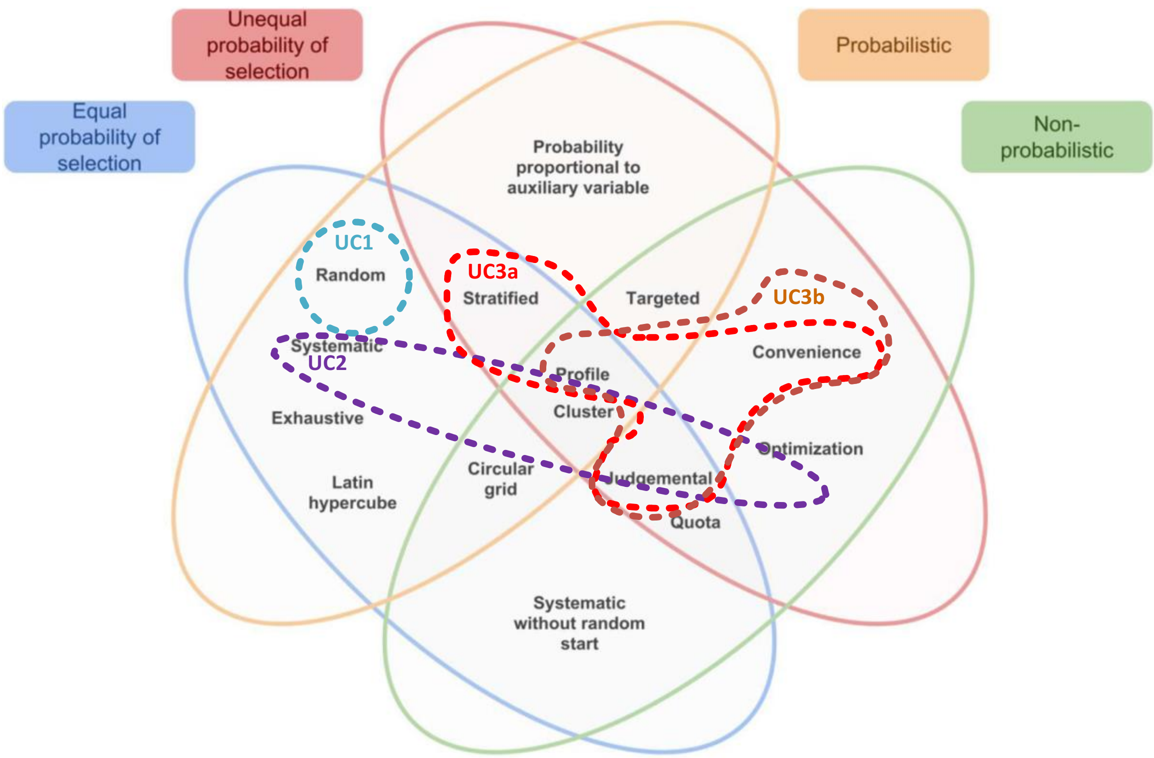

Figure 6: Visual representation of the sample design approaches applied in the different use cases

Data analysis methods

The STRATEGIST web tool foresaw some additional quality assurance/control checks on the existing data during the pre-processing step (e.g. errors, outliers, sample representativeness). However, the first version did not mention the use of **validation techniques for assessing the results** obtained. Both UC2 and UC3a show methods to assess the reliability of the data analysis process.

As illustrated in Figure 7, there is no unique solution to the data analysis method selection problem and in many cases various methods might be combined. In the case relevant physical processes can be simulated, the use of a sound process model may serve as additional data or trend model as shown for activation in UC3b.

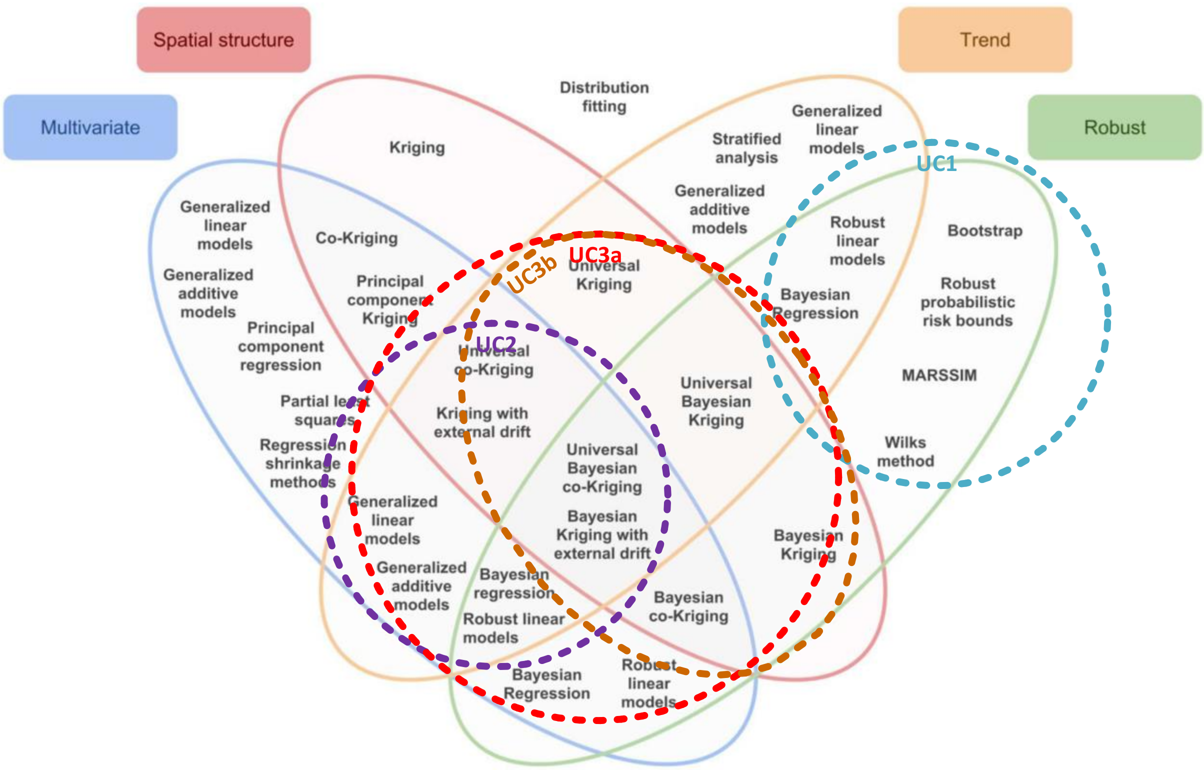

Figure 7: Visual representation of the data analysis methods applied in the different use cases

Uncertainties

Parameters influencing the uncertainty might depend on the physical quantity to be estimated (e.g. volume, activity concentration, total activity) and the required confidence level, but might as well strongly depend on objectives and sampling design. Some parameters can be more important than others. The return of experience from the three use cases regarding uncertainties is summarised as follows:

- The impact of the **sampling design** is most fundamental (see section on sampling design).
- Using advanced statistical methods for dealing with **samples below detection limit** can have an important (positive) impact on estimated values and should be considered in case the data set contains a considerable amount of results below detection limit (see section on overall strategy). Obviously, the potential impact depends on the objective (estimated quantity).
- Apart from the general aspects mentioned above, we also observe effects which could be occasionally generalised as well, but in other instances might be specifically related to the sampling design and data analysis implemented in the following use cases:
    - UC1: In the case of **small data sets**, the presence of **outliers** could clearly increase the uncertainty. Additional verification (process driven or error) might be necessary when estimations are becoming close to a decision threshold.
    - UC2: Sensitivity analysis shows that the most important uncertainties for the physical parameters estimated (e.g. volume categorisation, total activity), are due to **spatial uncertainty** (geostatistical simulations) and **heteroscedasticity**. Heteroscedasticity occurs more often in datasets that have a large range between the largest and smallest observed values, which is typically the case for radiological data. The contribution to the global uncertainty, resulting from measurement uncertainties on primary and secondary data, the relation between secondary and primary data, and the trend model are

relatively limited. Effects of heteroscedasticity on the uncertainty could be reduced using rescaling techniques or, in case sufficient data is available, sub-dividing the data in groups and applying data analysis on each group separately.

- UC3a: Sensitivity analysis shows that the **impact of sample measurement uncertainty** on the volume categorisation is **quite limited** (as it is in the case of UC2). The analysis shows as well that the effect on the estimated quantity (e.g. total activity or threshold) is not always the same as on the uncertainty. In addition, the integration of non-destructive measurements in a multivariate approach significantly reduces uncertainties when sampling is reduced.
- UC3b: The variance decomposition was fully possible and highlights that most of the uncertainty budget comes from the spatial distribution of values in comparison to the uncertainty related to sample duplicates and even more to measurement replicates. For one third of the radionuclides (Co-60, Ba-133, Eu-154 and Pu-239 + Pu-240), estimations without measurement uncertainty treatment are up to 95% less than estimations with measurement uncertainty treatment and for one third of the radionuclides (C-14, Cl-36, Eu-155 and Ni-63), estimations with measurement uncertainty treatment are up to 28% less than estimations without. That shows the impact of uncertainty is not negligible on final activity estimation in particular in the case of small datasets (less than 20 measurement data for 75% of the radionuclides).

Conclusion

A proper data analysis and sampling design strategy simplifies and optimizes the decision making process concerning the selection of the different D&D scenario options. We developed the STRATEGIST web tool to guide the expert in handling the problem definition and applying a data analysis and sampling design approach for initial nuclear state characterisation in view of decommissioning. The first version was adjusted and finalized, based on an extensive list of the lessons learnt from its implementation in four different use cases. It is only a guideline, however and should not be followed blindly. It provides the expert flexibility for the selection of methods. This is vital in view of the fact that the same problem can often be tackled using various methods. The STRATEGIST user-friendly web tool is freely available (INSIDER, 2019).

Acknowledgments

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Annex 1 : Main properties of the use cases and selection of sampling design and data analysis methods

	UC1	UC2	UC3a	UC3b
Subject	LLLW stored in two tanks	Biological shield of a PWR	Contaminated soil beneath a nuclear building	Graphite of a gas graphite reactor
History	Mixture of various R&D projects	Production of electrical power & reactor R&D	Radiochemistry on trans-uranium elements	Production of electric power and plutonium
Amount	100 m³	622 m³ (> 2000 tons)	up to 600 m³	about 580 m³ (1300 tons)
Objective	conformity with WAC (artificial)	categorization	Categorisation (average & total activity)	Categorization (radiological inventory)
Available data set (prior)	24 samples (12 for each tank)	184 primary & 58 secondary	223 samples from 7 horizontal cores at 2 depths	4 cores in 3D (> 20 samples)
Additional sampling	yes, but no impact on the sampling design	yes	no	no
Final dataset	same as prior (additional measurement results only used for QC)	834 (415 primary & 419 secondary)	same as prior	same as prior
Data analysis & sampling design				
univariate or multivariate?	univariate	Multivariate, but translated to the key nuclide approach	both	univariate
spatial trends?	no (initial sampling) maybe yes after sedimentation	yes	yes	yes
spatial structure?	no	yes (trend residuals)	yes	yes
robust methods?	yes	yes (robust model during data preparation)	yes	yes
sampling design probabilistic?	prior yes (additional samples no)	partly (also targeting/judgmental)	no	no
selection probabilities equal?	prior yes (additional samples no)	partly	no	no
selected methods for sampling design	prior: random (additional: convenience)	systematic & judgemental	convenience/judgemental	convenience/judgemental
selected methods for data analysis	bootstrap, Wilks, Bayesian, theoretical mean incl. uncertainty, LoD	log-log linear models, linear trend models, geostatistical methods (krigging & simulation)	geostatistical methods (krigging), probabilistic models (log normal fitting)	geostatistical methods (krigging), probabilistic models (log normal fitting)