

Soil and groundwater environmental data management and modelling for decommissioning of a nuclear site

GUIDELINES
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Foreword

In 2021, the European Commission (EC) adopted a new proposal for a Council Regulation¹ establishing a dedicated financial programme for decommissioning nuclear facilities and managing radioactive waste. This instrument covers the co-funding of the decommissioning programmes of Bulgaria, Slovakia, and the decommissioning of the Joint Research Centre (JRC). A separate Council Regulation² was adopted for the decommissioning programme of Lithuania.

The EC JRC is mandated to foster the spread of decommissioning knowledge across all the European Union Member States and facilitate knowledge sharing arising from implementing the abovementioned decommissioning programmes, funded by the Nuclear Decommissioning Assistance Programme (NDAP).

The decommissioning operators from the NDAP (NDAP Operators) implemented and tested a knowledge management methodology in 2021 through Project ENER/D2/2020-273. Using this methodology, the NDAP Operators can develop Knowledge Products that are currently available to share with other European stakeholders. In addition, this methodology is under implementation in the JRC Nuclear Decommissioning and Waste Management Directorate (NDWMD), which becomes a knowledge generator extracting the knowledge from the ongoing decommissioning activities at the different sites (Geel, Ispra, Karlsruhe, and Petten).

The JRC NDWMD aims to become a Centre of Excellence in nuclear decommissioning knowledge management and develop a decommissioning knowledge platform which allows exchanging information and building on the best practices in the EU inside the multi-annual financial framework (2021 – 2027) strategy. The operational phase of the project is expected to start in 2024 to develop ties and exchanges among EU stakeholders and document explicit knowledge and make it available through multi-lateral knowledge transfers on decommissioning and waste management governance issues, managerial best practices, technological challenges, and decommissioning processes at both operational and organisational level, to develop potential EU synergies.

This is a Knowledge Product prepared by the Nuclear Decommissioning and Waste Management Directorate (NDWMD) – Directorate J of the Joint Research Centre.

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¹ Council Regulation (Euratom) 2021/100 of 25 January 2021 establishing a dedicated financial programme for the decommissioning of nuclear facilities and the management of radioactive waste, and repealing Regulation (Euratom) No 1368/2013

² Council Regulation (EU) 2021/101 of 25 January 2021 establishing the nuclear decommissioning assistance programme of the Ignalina nuclear power plant in Lithuania and repealing Regulation (EU) No 1369/2013

PRODUCT DESCRIPTION

The knowledge product “Soil and Groundwater Environmental Data Management and Modelling for Decommissioning of a Nuclear Site” was prepared by a team of experts from [Ramboll Italy S.r.l.](#) and [NUVIA](#) at JRC Ispra Site *in the* Ispra Municipality (Province of Varese) in Italy. The guidance and recommendations of this knowledge product are collected from the experience gained during the execution of the “State-of-the-art Approach to Environmental Activities Related to Decommissioning of Nuclear Installations at JRC Ispra Site”, sponsored by the European Commission via the Nuclear Decommissioning Assistance Program (NDAP) between years 2020-2022.

The guidelines presented in this report aim to assist JRC Ispra personnel in making the decommissioning process of a nuclear installation and the management of contaminated soil by 3D modelling and simulation of contamination spreading, which is one of the activities in the frame of the pilot project of radionuclide contaminated soil management (Contaminated Soil Pilot Project), to develop a methodological approach on the environmental activities.

The user will find in the guidelines a methodology that can be followed in the management of the decommissioning of a nuclear installation and contaminated soil and groundwater, which can lead to the optimal management of the process through the acquisition of knowledge and techniques regarding the digital management of data and the creation of a geodatabase, the interpolation procedures and the creation of a site-specific conceptual model, and finally the 3D modelling of soil, subsoil and groundwater.

ABSTRACT

The guidelines presented in this knowledge product provide the Nuclear Decommissioning & Waste Management Directorate with technical guidance for developing a methodological approach to the environmental activities relating to managing contaminated soil and groundwater, using 3D modelling software and simulation of contamination spreading.

The first section describes digital data management and the creation of a geodatabase, which are fundamental elements for developing the subsequent phases. By analysing the data, the user can acquire basic information regarding the main existing interpolation techniques and their relative advantages and disadvantages to create a 3D conceptual model. Finally, through the present guidelines, the user can use tools relating to numerical models capable of simulating and determining the extent of contaminants and the risk they pose to receptors.

The results obtained are fundamental in securing and remediating the area of interest, on the one hand, allowing operators and technicians to monitor and manage potentially contaminated soil and water with more safety while allowing customers to reduce project costs because field investigations will be optimised.

OBJECTIVE

The main objectives of the present guidelines are to provide a process to determine whether a detailed evaluation of remediation options is necessary and, if so, guide a site-specific evaluation of the technical feasibility and cost of various remediation options. They consist of the following:

- Learning a methodologic approach for personnel not familiar with it and explaining its capabilities, including future capabilities foreseen by the developers.
- Acquiring a methodological approach to the environmental activities related to the decommissioning process of a nuclear installation, managing contaminated soil and groundwater data, and the 3D modelling and simulation of contamination spreading of radionuclide-contaminated soil and groundwater.

- Learning a methodological approach that allows correct and safer management of soil and groundwater potentially contaminated by radionuclides during decommissioning, using numerical models capable of simulating and determining the extent of contaminants and the risk they pose to receptors.

APPROACH

To develop these guidelines, the project team incorporated experience and lessons learned by Ramboll employees from a pilot project concerning potential soil and groundwater remediation during the decommissioning of a nuclear facility owned by JRC Ispra. The results were obtained by applying Ramboll's experience in the sector and acquiring new competencies in the modelling and interpolating process.

The old Liquid Radioactive Waste Treatment Station (STRRL, also known as Area 52) of the Joint Research Centre (JRC) [1] is not a high priority for decommissioning and hence was chosen as a candidate site for implementing the Contaminated Soil Pilot Project. The data acquired and the pilot test carried out, in parallel with the use of innovative software (3D modelling), made it possible to develop a methodology that would provide a guideline for future contamination activities and provide the essential data that allowed the elaboration of the present guidelines.

Specifically, the process and steps necessary to build a 3D model are described, and the available tools and methodology are explained. Finally, it explains how the 3D model can simulate pollutant transport phenomena, i.e., how contamination is distributed in soils and groundwater. The guidelines were developed based on Ramboll's experience to guide engineers and technicians dealing with radioactive waste disposal activities, even if they are not experts in the methodology described.

The presented methodologies can be further explored and applied, considering the relative advantages and disadvantages based on the tools introduced and briefly described in the present knowledge product.

RESULTS, FINDINGS, AND INSIGHTS

This document provides guidelines for data management and modelling of contamination in soil and groundwater at nuclear sites. The procedure for identifying and quantifying the contaminated area for remediation starts always with a study of the bibliography, records, documents and previous investigations of the affected site, then proceeds with establishing site investigation criteria, construction of a conceptual model, and finally, building a numerical model of contamination transport in case of a leak or spill. Applying the methodology described in the present knowledge product to the case of the Area 52 site of the JRC, the following considerations should be included in the procedural process:

- Potential for off-site migration of contamination following an unintentional release.
- Potential impact on decommissioning planning and costs, such as the disposal of contaminated materials from decommissioning of which soil could represent the biggest volume.
- Limitation of risks by decreasing the time of potential exposure to radiation from radionuclides.

An important recommendation concerning the availability of baseline data and preparatory information is that intrusive investigations in such areas should be preceded by archive documentation study searching for sub-surface services, or search activities should be carried out using specific tools.

TARGET USERS

The users who will benefit from the guidelines presented in this document are Nuclear Decommissioning & Waste Management Directorate (ND&WMD) operators involved in environmental monitoring and managing soil and water potentially contaminated with radionuclides.

Specifically, the guidelines can help the senior technical workers who deal with the radioactive waste disposal activities to manage the remediation project through the approach described, which allows to limit costs and risks in the field; on the other hand, the junior technical figures (geologists, engineers, radiologist or technicians) who acquire data in the field, will benefit from the fact that the guidelines can provide a method that reduces exposure to contamination in the data collection stage.

Furthermore, among the possible positive consequences of implementing the actions described, it is highlighted that they will bring an economic advantage to both the customer and the manager of the on-site investigation activities, as the latter will be considerably optimised.

APPLICATION, VALUE, AND USE

The guidelines presented in this document can be used by any nuclear decommissioning organisation facing contaminated soil problems and willing to implement an innovative digital method involving 3D modelling software.

Supposing the user is faced with a contaminated soil or water problem, the present knowledge product can be used directly, considering that for its implementation, it will be necessary to evaluate the following aspects:

- The guideline requires using 3D modelling software and personnel trained in using such software.
- The analyses and surveys needed to characterise the study area will only be mentioned broadly. Additional tests and analyses may be necessary depending on the specific case (reference is made to technical norms and national legislation for more information).

The guidelines' content is based on experience, which shows that they can allow operators to carry out the data acquisition phases more efficiently and expose themselves to less risk. Thus, the entire remediation project can be implemented more efficiently.

If followed, the guide can provide a supporting tool that can be implemented and adapted to different situations and cases located in different sites and affected by different types of contamination.

As seen, the knowledge product can provide support and make the process safer, more efficient, and more economical. Multiple operators can apply this, obtaining tangible advantages in terms of time, efficiency, and costs.

KEYWORDS

DECOMMISSIONING, CLEANUP, DECOMMISSIONING, CHARACTERIZATION, SITE CLEANUP.

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LIST OF ACRONYMS AND DEFINITIONS

3D	Three-Dimensional
CSM	Conceptual Soil Model
DTM	Digital Topographic Model
EC	European Commission
IDW	Inverse Distance Weighted
JRC	Joint Research Centre
ND&WMD	Nuclear Decommissioning & Waste Management Directorate
NDAP	Nuclear Decommissioning Assistance Program
REV	Representative Elementary Volume

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1. BACKGROUND

The guidelines present a method to analyse the site, creating benefits for stakeholders (ensuring the optimization of data management, increasing safety through reduced exposure to contaminants, improving the efficiency in process management, and also providing economic benefits). The guidelines can provide a supporting tool that can be implemented and adapted to different situations and cases located in different sites and affected by different types of contamination.

This document aims to guide personnel involved in nuclear decommissioning projects towards a greater understanding of:

- A methodological approach to environmental and monitoring activities for managing contaminated soil and groundwater.
- An understanding and knowledge of the use of software, including 3D data management and modelling software, helpful in understanding the potential in the field of potentially contaminated water and soil management.

The method aims to create practical guidance applicable to many workers and radionuclide-contaminated sites. It enables proper, safer, and more efficient management of potentially radionuclide-contaminated soil and groundwater during decommissioning using numerical models that can simulate and determine the extent of contaminants and the risk they pose to receptors and operators.

1.1. Relevance

Based on the experience described, the following impacts have been observed, involving both workers and stakeholders interested in the project (and which, it is believed, can be extended to similar application cases in future):

- Optimised management of data in up-to-date and updatable versions.
- Increased safety through reduced exposure to contamination at a nuclear site.
- Increased efficiency in contamination management.

Finally, the method presented below can be applied to many cases because the accuracy of site modelling and characterisation is independent of the type of radionuclide found at the site or its geomorphological characteristics.

2. SCOPE OF THE TRAINING

The present knowledge product has been developed based on the experience gained by the Ramboll's team to define and describe a methodological approach to the environmental activities related to the decommissioning process of a nuclear installation and the management of contaminated soil and/or groundwater and on the 3D modelling and simulation of contamination spreading of radionuclide-contaminated soil and groundwater.

The guidelines provide valuable tips for personnel unfamiliar with software that allows them to carry out 3D modelling and data management. The primary learning objectives of this training are the following:

- To explain the software capabilities, including foreseen features.
- To allow correct, more effective, and safer management of soil and groundwater potentially contaminated by radionuclides during decommissioning, numerical models capable of simulating and determining the extent of contaminants and the risk they pose to receptors will be used.

3. METHODOLOGY AND DATA MANAGEMENT

The methodological approach to the environmental activities related to the decommissioning process of nuclear installation and the management of contaminated soil and/or groundwater proposed in this knowledge product includes the following steps (Figure 1):

1. Data analysis and proposal of the investigation plan.
2. Execution of on-site additional investigations.
3. Development of the final conceptual model of soil and subsoil.
4. 3D modelling (of both unsaturated and saturated soils).

The guidelines analysed the above steps, dividing them into four distinct phases that are closely related, as described below. The work environment and the preliminary characterisation of the area of interest are explained in Section 3.1. The description of the construction of the conceptual model, starting from the data analysis and the data management, is depicted in Section 3.2. Reference is made to Section 3.3 for details regarding how to run an interpolation and which type is suitable for specific data. The fourth and final step, to which Section 3.4 is dedicated, describes how to run a contamination transport model.

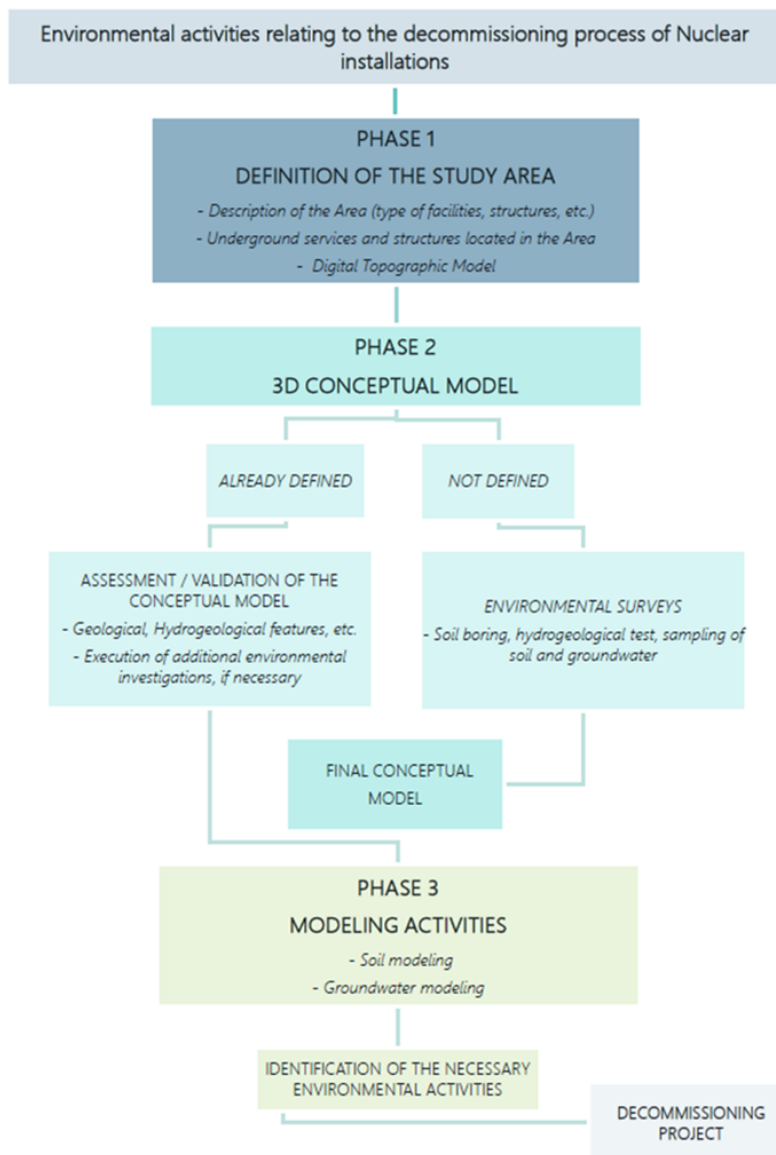


Figure 1: Methodological approach including the associated environmental activities.

3.1. Environmental Data Collection

The definition of the area of study starts based on the available existing bibliography and data regarding these aspects:

- Description of the facilities, structures, location of underground services and structures in the area: to complete this activity, data relating to site plans are acquired, and information is sought on the structures in the study area and surrounding areas (e.g., location of the sewage network, presence and location of the electricity network, and other utilities, distance from the study area, and, if available, materials of which they are composed). This information can be found through an initial archives survey and by requesting data from the current site owners. For example, the site owner can request the structure plan or the sewer system directly, indicating the diameter and material with which the pipes were built and at what depth they are located. In addition, evidence of the current activities on the site can be requested.
- Historical operations and production processes: Historical information is sought on the site's previous arrangements and activities to investigate the presence of possible sources of past contamination. If information cannot be found online or in the archives, surveys or interviews with previous owners of the area may be necessary.

Digital Topographic Model (DTM) of the study area. The DTM represents the distribution of the quotas of a territory or surface in digital format. The digital elevation model is generally produced in raster format by associating the attribute relating to the absolute elevation to each pixel. The DTM can be made using different techniques; the most sophisticated models are generally created using remote sensing techniques. These involve processing data acquired through a satellite, aircraft, or ground station sensor. Such data are usually made public through *webgis* (a technology used to display and analyse spatial data on the Internet), including the study area. If there is not enough specific data available online (or if the resolution is lower concerning our purpose), the DTM can be obtained through a topographic survey (which requires the use of special equipment and specialised personnel) or using drone surveys (which also require the presence of personnel trained on the use).

In this phase, the environmental information related to the area of interest may be mapped within a Geodatabase. A Geodatabase is a database that collects all information, not only alphanumeric but also geographical, of physical objects of interest; it therefore allows geo-reference of the data collected. The data is collected in the geodatabases using software with the following characteristics:

- It should be a valid, adaptive, upgradeable, and easy-to-use tool, which allows the simple and efficient management of environmental data, ensuring:
 - Easy acquisition of environmental data.
 - Reliability and data quality verification.
 - Storage security.
 - Easy access to the database.
 - Speed and ease of analysis.

In the study case described, a geodatabase is a fundamental tool that stores all the information about the site, lithology, and groundwater measures. The option of a “live” database (updatable on-site, e.g., with a tablet or a mobile device app) should be considered.

The characterisation of the environmental setting consists of defining the preliminary conceptual model of the area, i.e., based on bibliographic knowledge, the principal geological, geomorphological, hydrogeological studies and bibliographic information, the study area is defined. The following are the aspects to be considered:

- Geological and Geomorphological Description.
- Litho-Stratigraphic Profile.

- Soil characteristics (density, porosity, etc.).
- Hydrographic (surface water) and hydrogeological characteristics (permeability, groundwater level, etc.).
- Chemical and radiological characterisation of soil and groundwater.
- Soil surface recharge – hydrogeological balance.

To prepare the preliminary conceptual model, any investigations conducted in the various environmental matrices during the site's management before implementing the investigation plan should be considered [2].

The preliminary conceptual model allows the user to define the areas for which a deeper detail will be necessary by performing new environmental investigations focusing on soil, subsoil, and groundwater (in the subsequent phases). This process will guide the definition of the investigation plan.



The most critical issue is knowing the site and studying all soil and groundwater characteristics.

3.2. Characterization of the Study Area and Data Management

The purpose of this phase is to characterise the soil, subsoil, and groundwater of the area of interest, which were only preliminarily defined in the previous phase through the available desktop data. To do this, an **Environmental Investigation Plan** will need to be prepared, which consists of a plan that describes which characterisation activities are to be performed and with which methods and frequencies. The objectives of the plan are the following:

- Verify the accuracy of all the data gathered during the environmental data collection.
- Incorporate updated information from the on-site observation.
- Define a specific site conceptual model, which consists of an updated version of the preliminary conceptual model, updated through the specific data acquired in the field.

A **digital approach** to the survey implementation should be used during this phase. Through digital data collection, it is possible to optimise the operations in the field, and it provides an efficient method for collecting data faster and more accurately. The method facilitates data collection, entry, and analysis. It can ensure efficiency and accuracy. Digital data collection also offers data quality by allowing skip patterns, entry limits, and geotagging to capture respondents' locations. It ensures the safety of the data since they can be sent directly to a secure server without risks of getting damaged. Using a digital approach ensures the following advantages:

- All the gathered data are digitised directly in the field (e.g., with a tablet for on-site use or with an app on mobile devices).
- Accurate geo-referenced field data are captured and returned.
- Documents and photos for any observation/test made on-site are uploaded in the geodatabase directly on the field.
- Data are directly stored from the field.
- It is possible to access data analysis and visualisation via web-based reporting tools.
- Viewer with simple user interfaces for viewing maps.
- Access to data from anywhere (office, field) via browser or app.
- Efficient data sharing and direct collaboration with the team.

Numerous digital data acquisition software exists, with different characteristics: free or paid, more intuitive or which may require training, with more or fewer functions, etc. The requirements of the work to be done and the environmental context should be considered when choosing the software that allows data collection digitally more efficiently.

Once the software is chosen, the following aspects should be considered to ensure the data is properly collected:

- Understand correctly how to apply it to the project. Many tools need specific training and consultations for their usage.
- Execute the software properly; comprehensively understand the project's end goal before collecting data.
- Ensure the data will be centrally available: One of the most significant advantages of digital data collection is the ability to share information in real-time, so it is important to make the data central and accessible to the project teams to save time and effort.
- Ensure to have the right team for the job, eventually providing training to the team's members on using tools and software.
- Understand how to perform quality control on the data: consistency quality assurance is essential, not to waste time and effort.

A methodological approach enables the development of an adaptive and dynamic tool. That is, the system can be improved iteratively during the described procedures. The activities within the Environmental Investigation Plan include hydrogeological and geological surveys, water, groundwater, and soil samples. They aim to characterise the study area by following national and international laws and guidelines.



The most important issue is understanding the need to carry out appropriate characterisation surveys and carefully define such environmental surveys.

3.3. 3D Conceptual Model

A conceptual soil model (CSM) is an iterative tool that should be developed and refined as information is obtained during the site history review and continues throughout the site and/or remedial investigation. A CSM aims to describe relevant site features and the surface and subsurface conditions to understand the extent of identified contaminants of concern and their risk to receptors.

The CSM can be presented in several forms. Often, the forms will be dictated by the complexity of the site or area of concern and the amount and type of available data. The CSM may be narrative, text, pictorial, presented as a computer model, or some combination. It should represent the site or area of concern, contaminant sources, the environmental media that have been impacted, and the processes that determine the transport of contaminants to potential receptors. Refine the CSM as information is collected throughout each project phase until a remedy. A CSM is also helpful after implementing the remedy [3].

Following the leading national and international guidelines, given a possible contamination scenario, the following aspects should be identified and described to develop the conceptual model of the site:

- Geological features of the site.
- Hydrogeological features of the site.
- Characteristics of the "source areas" of potential contamination based on the results of characterisation surveys.

Starting from the data generated by previous surveys (e.g., the stratigraphic log), it will be necessary to provide for processing this information through data interpolation. Often, a limited number of data obtained through sampling or measurement equipment is available. It is needed to identify a function that links all the data available and can be used to identify new points in the set of collected data. In the case of geological data, the depths of the various layers detected in each borehole analysed, if interpolated, allow us to recreate the stratigraphic structure of the site.

Interpolation is helpful for various purposes, such as filling in missing data, smoothing noisy data, and forecasting future trends. It can also help to understand the underlying patterns and relationships of the data and test different hypotheses and models. However, it has some limitations and assumptions that the user needs to be aware of [4]. Assumptions should be related to such characteristics as:

- The domain’s hydrogeology, stratigraphy, etc.
- The dimensionality of the model (one, two, or three dimensions) and the geometry of the boundary of the domain of interest.
- The behaviour of the system: steady state or time-dependent.
- The kind of soil and rock materials comprising the domain and the inhomogeneity, anisotropy, and deformability of these materials.
- The number and kinds of fluid phases (e.g., water, air, contaminant) and the relevant chemical species.
- The extensive quantities transported within the domain.
- The relevant material properties of the fluid phases (density, viscosity, compressibility, presence of solutes).
- The relevant transport mechanisms within the domain.
- The possibility of phase change and exchange of chemical species between adjacent phases.
- The relevant chemical, physical, and biological processes in the domain.
- The flow regimes of the involved fluids (e.g., laminar or non-laminar).
- The existence of non-isothermal conditions and their influence on fluid and solid properties and chemical–biological processes.
- The assumed sharp macroscopic fluid-fluid boundaries, such as a phreatic surface.
- The relevant state variables and the areas or volumes over which averages of such variables should be taken.
- The sources and sinks of fluids and contaminants within the domain and their nature (spatial distribution and temporal variation).
- The initial conditions within the domain and conditions on its boundaries.

There are many interpolation methods, depending on the type and shape of the data and the desired accuracy and complexity. The most common methods are linear, Kriging, Inverse Distance Weighted (IDW), Polynomial regression, Spline regression, kinematic, and Bézier curve. Table 1 summarises the advantages and disadvantages of using interpolation methods.

Table 1: Advantages and disadvantages of using interpolative methods

Advantages ⊕	Disadvantages ⊖
<ul style="list-style-type: none"> ▪ Allow for estimating values that are not directly observable or measurable or are too costly or time-consuming to obtain. ▪ They can help fill in the gaps in the data and make it complete and more consistent. ▪ Interpolation techniques make data more suitable for analysis and visualisation. ▪ They can help create curves and surfaces to represent the data accurately. 	<ul style="list-style-type: none"> ▪ They are based on assumptions and approximations that may not reflect the reality of the data. ▪ It is possible to introduce errors and uncertainties in the estimated values, especially when the data is noisy, sparse, or extrapolated far beyond the data range.

Acquiring experimental data that will be used to interpolate or extrapolate to understand the nature of the data is important. Interpolating data can be done with greater confidence so long as the data was acquired with sufficient regularity to understand both the data's trends and variability due to experimental uncertainties.

The selection of the interpolation method depends on several factors, such as the data's type and shape, the estimation's purpose, and available resources. The following four factors are the most relevant:

- The objective(s) of the investigations, i.e., what information is required to provide for the purpose (rough preliminary estimates vs. more detailed predictions).
- The available resources required to construct and solve the model. Included are the availability of expertise, skilled personnel, and computers to describe processes and the availability of field data required to validate the model and determine the numerical values of its coefficients.
- The legal and regulatory framework which pertains to the considered case.
- The objectives of an investigation dictate which features of the domain and its behaviour should be represented and to what degree of accuracy and detail.

A more detailed conceptual model requires more field measurements to calibrate it. Data acquisition is usually more expensive than code and computer costs.

The most important step in the modelling process is selecting the appropriate conceptual model for a given problem. If the model is oversimplified, the required information can probably not be produced. If it is undersimplified, the information needed for model calibration and coefficient determination cannot be obtained (as the resources to solve the model). If inappropriate or wrong assumptions are selected, the model may not represent the system behaviour features relevant to the management problem at hand.

One essential part of the CSM is the surface contamination layer. This can be built upon surface contamination measurements and interpolation methods. Most interpolation methods can create prediction surfaces, the default output of all interpolation methods. This surface displays the predicted value of the data at all locations between the measured locations, obtaining the final 3D conceptual model of soil, subsoil, and groundwater.



It is best to choose an interpolation method that matches the nature and behaviour of the data to avoid overfitting or underfitting. A specialised technician should make this choice. The method should minimise the error and uncertainty in the estimated values while providing a measure of confidence or error bounds. Lastly, it should be flexible and adaptable to handle different scenarios and conditions.

Among the various interpolative methods, the most used are:

- Kriging, also known as Gaussian process regression, is a method of interpolation based on the Gaussian process governed by prior covariances.
- Inverse Distance Weighted (IDW): is a simple technique for curve fitting, assigning values to unknown points by using values from known points.
- Polynomial regressions: This method creates a floating-point grid by using polynomial regression to fit a least-square surface to the input points.
- Spline regressions (Regularized & Tension) are a form of interpolation in which the interpolant is a special type of piecewise polynomial called a "spline." Spline interpolation is preferred over polynomial interpolation because the interpolation error can be made small when using low-degree polynomials for the spline. Cubic spline interpolation is a special case for Spline interpolation; it is piecewise cubic and twice differentiable over the entire interval.
- Bézier curve: a parametric curve used in computer graphics and related fields; discrete "control points" define a smooth, continuous curve employing a formula.
- Kinematic: incorporates object kinematics (i.e., velocity and acceleration) into the interpolation process.

Table 2 summarises the advantages and disadvantages of the most popular interpolation methods.

Table 2: Comparison between different interpolative methods [5] [6]

Interpolative Method	Advantages ⊕	Disadvantages ⊖
Linear	Quick calculation No overshooting No ondulation	Inaccurate interpolation (Non-linear movement)
Cubic spline	Stable Less computation	Overshooting problem
Polynomial	Simple calculation	Expensive computing Undulation problem
Bézier curve	Simple calculation Effective interpolation (Non-linear movement)	Sampling points decision problem
Kinematic	Effective interpolation (Fast-moving or linear movement)	Inaccurate interpolation (Large spatial movement)
IDW	Wide application range and fast calculation speed	Can produce bullseyes around data
Kriging	Predictions based on a spatial statistical analysis of the data. Best linear unbiased estimator Many forms are available, applicable to various data configurations. Automatically accounts for clustering and screening effects; remains efficient in sparse data conditions. Can consider variation bias toward specific directions (anisotropy) Able to quantify interpolation errors (Kriging variance)	Overall complexity Requires care when modelling spatial correlation structures. Assumptions of intrinsic stationarity may not be valid (drift) and be handled through an appropriate Kriging variant. Most Kriging variants are exact (no smoothing) More computationally intensive than other local methods

The use of the Kriging interpolation method is suggested for the present application. Kriging assumes that random processes with spatial autocorrelation can model at least some of the spatial variation observed in natural phenomena and require that the spatial autocorrelation be explicitly modelled. Kriging techniques can describe and model spatial patterns, predict values at unmeasured locations, and assess the uncertainty associated with an expected value at unmeasured locations. Ordinary kriging assumes the model:

$$Z(s) = \mu + \varepsilon(s)$$

Where μ is an unknown constant, one of the main issues concerning ordinary Kriging is whether the assumption of a constant mean is reasonable. Sometimes, there are promising scientific reasons to reject this assumption. However, as a simple prediction method, it has remarkable flexibility.

All interpolation models are predictive methods, and the goal is to produce a surface of predicted values at all locations between the measured locations.

Frequently, the geostatistical analysis offers several different output surface types to help interpret the prediction surface while considering the predictions' inherent variability to understand how precise and reliable they are.

All output maps assume you have chosen the correct interpolation method and interpolation parameters. In practice, if the data does not meet the assumptions of the interpolation method or the wrong parameters are supplied, these surfaces may not correctly represent the true values of the data.

Another sound output is the **prediction standard error surface**, which maps the standard errors of the predicted values at each location. Standard errors are the standard deviation of the estimated value, and the larger the standard error, the lower the precision of the predicted value. Standard errors are often used to create confidence intervals for the predicted values. Standard error values should be interpreted while keeping in mind the values and range of the input data. For example, a standard error of around 1 % is considered high precision. Standard errors of around 50 % are regarded as low precision because the variability of the predictions is of the same magnitude order as the input data.

Figure 2 below shows an example of the Kriging algorithm's graphical results.

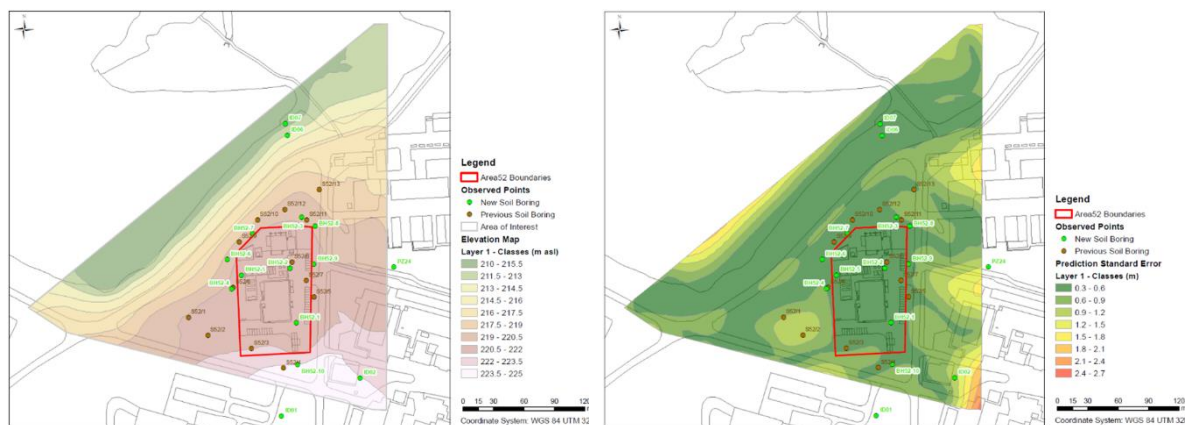


Figure 2: Examples of the outputs of the elaborations of the Kriging algorithm: spatial pattern and predicted standard error.



The most important decision made very early in developing a CSM is the selection of appropriate temporal and spatial scales of data collection, both regional and local (site-specific).

3.4. Modelling Activities

The use of modelling in the decision-making process can bring numerous advantages; models consist of useful tools in the case of studying a complex system (which generally corresponds to the environment analysed in a project), where outputs and results cannot be anticipated based on experience or available information. Management means making decisions to achieve goals without violating specified constraints. Therefore, good management requires information on the response of the managed system to proposed activities. This information enables the planner, or the decision-maker, to compare alternative actions, select the best one, and ensure that constraints are not violated. All such predictions can be obtained within the framework of a considered management problem by constructing and solving mathematical models of the investigated domain and the flow and solute transport phenomena that occur in it.

For most practical problems, it is impossible to solve the mathematical models analytically because of the heterogeneity of the considered domain and the irregular shape of its boundaries. Instead, the mathematical model is transformed into a numerical one that can be solved using software.

Figure 3 below reports a scheme of the significance of models when used in decision-making processes. The figure shows how implementing a model involves a monitoring phase that allows the process to be iterative to continuously improve the decision-making process with the results of consecutive iterations.

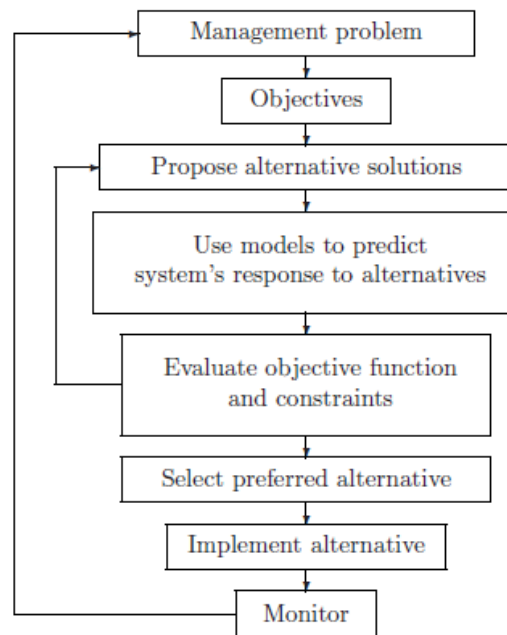


Figure 3: The role of modelling in the decision-making process [7]



Modelling activities can correctly represent the site only if the modeller knows what to expect.

3.4.1. The modelling process

The modelling process described in this subsection is summarised in Figure 4. It involves the following steps, which are further described in detail in the present sub-section:

- 1 Identification of the information required for making management decisions
- 2 Development of a CSM
- 3 Development of a mathematical model
- 4 Development of a numerical model and code
- 5 Code verification
- 6 Model validation
- 7 Model calibration and parameter estimation
- 8 Model application
- 9 Sensitivity analysis
- 10 Stochastic analysis
- 11 Summary, conclusions, and reporting.

Step 1: Identification of the information required for making management decisions

As emphasised above, models are needed to predict the outcome of implementing management decisions. To select the most desirable plan, the decision maker needs to assign values to a set of measures used to evaluate the success of a selected plan in achieving the desired objectives. The cost of a project, the period required for remediation, the quality of water reaching an underlying aquifer, and the quantity and quality of water that can be pumped from a considered aquifer may serve as examples of such measures. The actual values of the various measures depend on the managed system and its response to implementing a proposed plan. These, in turn, are used to evaluate the criteria, or objective function, employed for selecting the preferred management alternative. Information of this kind may also be required to ensure that a proposed alternative does not violate constraints imposed on the managed system. Constraints include regulatory limits on contaminant concentrations and the leakage to an underlying aquifer.

Step 2: Development of a conceptual model

Gathering information is always costly, so a balance should be sought between the additional information and the benefits to be gained from it. Modelling simplifies the system's description and behaviour to the degree that it helps plan and make management decisions in specific cases. For further details on this topic, refer to Section 3.3.

Step 3: Development of a mathematical model

In this step, the conceptual model is expressed as a mathematical model. The continuum type of model is usually (but not always) employed. The mathematical model consists of:

- A definition of the geometry of the surfaces that bound the domain.
- Equations that express the balances of the relevant extensive quantities (e.g., mass of fluids, mass of chemical species, energy).
- Flux equations that relate the extensive quantities' fluxes to the problem's relevant state variables (e.g., Fick's law for the diffusive mass flux of a chemical species in a fluid phase).
- Constitutive equations that define the behaviour of the phases and chemical species involved (e.g., the dependence of density and viscosity on pressure, temperature, and solute concentration).
- Sources and sinks of the relevant extensive quantities are often called forcing functions.
- Initial conditions that describe the known state of the system at some initial time.
- Boundary conditions that describe the interaction of the domain with its environment (i.e., outside the delineated domain) across their common boundaries.

In a continuum model, a partial differential balance equation describes the behaviour at every point within the domain. However, sometimes, we are not interested in what happens at every point. Instead, we need information on the lumped or averaged behaviour of an entire domain or parts of it. Another kind of model is called for in such cases, referred to as a lumped parameter model, a compartmental model, a multi-cell model, or an input-output one. In such a model, balances of the relevant extensive quantities are stated for 'cells' of different shapes and sizes of the domain; state variables are averages over these cells. Sometimes, the heterogeneity of a domain is such that an appropriate representative elementary volume cannot be found for it, and the continuum approach cannot be applied. A lumped parameter model may be required.

The core of any transport model on an extensive quantity is the balance equation of that quantity, for example, the mass of a fluid phase and the mass of a liquid phase component. In passing from a model at the microscopic scale to the macroscopic scale model, various coefficients of transport, transformation, and storage of the extensive quantities are introduced by some averaging process. The permeability of a porous medium, moisture diffusivity, and dispersivity are examples of such coefficients:

- The **permeability** is a measure of the flow resistance, which is exerted by the solid matrix (the soil element considered) on the free fluid flowing through a cellular biological medium and depends strongly on the detailed geometry and topology of the pore structure (i.e., the space allocated to free fluid). Typically, the hydraulic permeability of a cellular biological medium is obtained experimentally, with suitable experimental methods being different for various types of cellular biological media.
- **Diffusivity** is defined as the ratio of the molar flux to the corresponding concentration gradient; the diffusivity of a component expresses its mobility characteristic, and it is a function of temperature, pressure, nature, and concentration of the components.
- Lastly, the **dispersivity** expresses the effect on the flow of the microscopic configuration of the interface between the considered fluid phase and all other phases considered. This interface is between the fluid and the solid in a saturated system.

Permeability and dispersivity of a phase are examples of coefficients that express the macroscopic effects of the microscopic configuration of the boundaries between a considered phase and all other phases present in a representative elementary volume (REV) of the medium.

It is essential to realise that the coefficients derived by field experiments, in which (in principle) we compare measurements of certain state variables with the corresponding values predicted by a model, correspond to that particular model. If possible, one should not employ coefficients derived from one model in another one. When the coefficients developed for one model are used in another, errors may result. The magnitude of the error will depend on the differences between the two models.

In principle, to employ a particular model for a specific domain, the values of the coefficients that appear in the model should be determined from field experiments conducted in the domain. Typically, such an experiment involves comparing actual field observations and predictions made by the model, employing some parameter identification technique.

Step 4: Development of a numerical model and code

Having constructed a mathematical model regarding relevant state variables, it has to be solved for cases of interest. The preferred method of solution is the analytical one, as it provides a general solution (for a given domain geometry) that can apply to various sets of domain and fluid parameters.

However, because of the complexity of most problems of practical interest (shape of domain boundaries, heterogeneity, nonlinearity, irregular source functions, etc.), it is impossible, in general, to derive analytical solutions for them. Numerical methods are usually employed to solve the mathematical model. This means that various methods transform the mathematical model into a numerical one, in which their numerical counterparts represent the partial differential equations. A computer program or a code is required to solve the numerical model.

There is often no need to develop a code to solve a given problem, as such code is readily available, either as a public domain code or a commercial one that must be purchased. In most cases, buying a code is much cheaper than developing one. Codes are available for flow problems and most contaminant transport problems in single-phase flow, some with chemical and biological reactions and transformations.

Step 5: Code verification

When a new numerical model and a code are developed for solving a mathematical model, the code is not considered ready for use unless it undergoes a proper verification procedure. Here, verification means checking that the code does what it proclaims to do, namely, to solve the mathematical model. Verification involves comparing solutions obtained using the code with those obtained by analytical methods whenever possible. This is usually done for simplified domain geometry, homogeneous materials, etc. In many cases, analytical solutions cannot be derived.

The only procedure, then, is to compare code solutions with solutions obtained by other codes. Good codes, especially commercial ones, should have documented code verification.

Step 6: Model validation

Once a model has been selected for a particular problem in a specific site, it must be validated. Model validation ensures that the model correctly describes all the relevant processes that affect the excitation-response relations of interest to an acceptable degree of accuracy. The only way to validate a model is through an experiment.

Although it is desirable to perform the model validation for the actual site of interest, the model is often validated in principle, i.e., ensuring that it represents the phenomena by conducting controlled field or laboratory experiments. Unlike laboratory experiments, many features encountered in field experiments, such as heterogeneity and anisotropy, cannot be controlled or identified. Unfortunately, in many cases, they dominate the system's behaviour.

If model validation cannot be implemented, it is sometimes combined with model calibration.

Step 7: Model calibration and parameter estimation

We use model calibration for the activity that combines model validation and parameter estimation at a specific site of interest. These activities are executed simultaneously. Thus, in the calibration procedure, the values of model coefficients for a site are determined by solving an inverse problem using field data from that site.

In principle, the only way to obtain the values of these coefficients for a model of a considered domain, e.g., an aquifer, is to investigate the domain itself. Historical data are reviewed to find a period in the past for which information is available on initial conditions of the system, excitations of the system in the form of pumping, natural replenishment (infiltration from precipitation), the introduction of contaminants, or changes in boundary conditions, and observations of the response of the system, in the form of temporal and spatial distributions of state variables, e.g., moisture content and solute concentrations. Suppose such a period (or periods) is found. In that case, the known initial conditions and the known excitations of the real system on the model are imposed, and the latter's response to these excitations is derived. We must assume some trial values of the sought coefficients to derive the model's response. We then compare the observed and modelled responses. The desired values of the coefficients are those that would make the two sets of values of state variables identical. The measured response is compared with model predictions.

Various techniques exist for determining the 'best' or 'optimal' values of these coefficients, i.e., values that will make the predicted and the measured ones sufficiently (or acceptably) close to each other. The values of the coefficients eventually accepted as 'best' for a considered model depends on the criteria selected for 'goodness of fit' between the observed and predicted values of the state variables. These, in turn, depend on the objective of the modelling. Some techniques use the basic trial-and-error approach, while others employ more sophisticated optimisation methods. In some methods, a priori estimates of values to be expected for the coefficients, as well as information about lower and upper bounds, are introduced.

In addition to model calibration, or solving the inverse problem for the considered domain, model coefficients and parameters can also be estimated from:

- Literature survey.
- Laboratory experiments.
- Small-scale field experiments.

Step 8: Model application

The model is ready for use once a model has been calibrated for a considered problem (including all the required site-specific coefficients and parameters). Computer runs are then conducted to provide the required forecasts.

Step 9: Sensitivity analysis

The term sensitivity analysis describes tools that help the modeller evaluate the impact of uncertainty in the values of model coefficients on the results predicted by the model. Briefly, we want to know how sensitive the predicted values are to changes in the values of model coefficients. If these effects are not significant (from the point of view of the decision maker, who uses these predictions in the management process), we can accept the predicted values and make decisions.

If, however, the predicted values are sensitive to changes in parameter values, we must reduce the range of uncertainty in the values of these parameters. In most cases, we must invest more resources to acquire more accurate data. Sensitivity analysis can also assess the reliability of parameters determined during calibration. A residual error is usually expressed in the calibration process, e.g., as the sum of the squared differences between the measured and the predicted water levels. The optimal set of model parameters minimises this error. If a slight change in a parameter causes a significant change in the residual error, we may say the residual error is sensitive to that parameter.

Step 10: Stochastic analysis

The sensitivity analysis provides a qualitative description of uncertainty. It addresses questions like ‘What if there is 20% uncertainty in this parameter or that condition?’; it does not express the range of uncertainty in either the input or the output in terms of statistical measures, such as mean and standard deviation.

Step 11: Summary, conclusions, and reporting

The summary and conclusions should include the information that the model was expected to provide, as well as additional information concerning the accuracy of the information, the uncertainty involved, and suggested follow-up work.

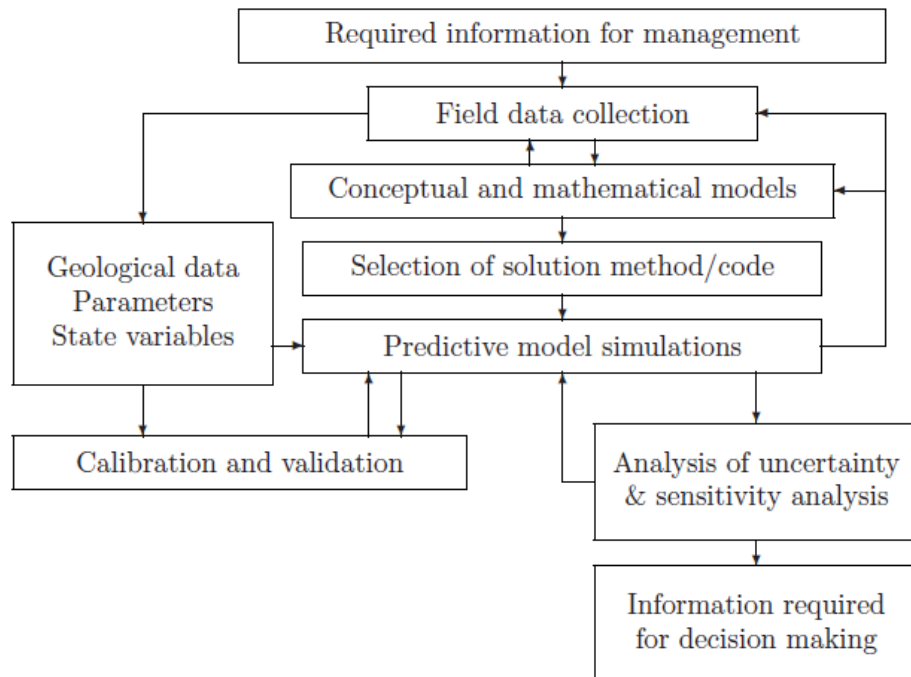


Figure 4: The modelling process [7]

Choosing the model type and the calculation code is crucial in modelling a hydrogeological system. This choice is based essentially on data availability, the system's complexity and the model's end use.

Excluding the physical models, for hydrogeological modelling, mathematical models are usually used to indirectly simulate water flow through equations suitable to represent the physical processes occurring in the system and equations that describe the loads and flows along the hydrodynamic limits of the model. In detail, the choice is limited to two types of models:

- **Analytical models:** These models are based on the existence of a direct mathematical solution of the equations of the investigated system, such as Darcy's law. This model type is reserved for simple cases or preliminary assessments of the problems under consideration. Still, it is unsuitable for complex cases with varying hydrogeological parameters in space and time.
- **Numerical models:** These models are based on the resolution of a set of differential equations associated with specific boundary conditions, representing water flow in an aquifer body. The solution to these equations consists of the distribution in space and time of the unknown function, such as the hydraulic load. Numerical models, therefore, require in-depth knowledge of the hydrogeological system and greater computing power to solve the differential equations that describe the flow.

The advantages and disadvantages of analytical and numerical models are summarised in Table 3. The following paragraphs will explain how 3D models can be used specifically in the case under study, i.e., the reconstruction of contamination in saturated and unsaturated soils.

Table 3: Comparison between analytical and numerical models (advantages and disadvantages)

Analytical models	Numerical models
Advantages ⊕	
Easy to use	Allow to represent complex systems.
A limited number of input parameters	Allow to represent multi-dimensional systems.
	Complex boundary conditions
	Consider the spatial variability of input parameters.
	Possible to consider stationary and non-stationary conditions
	Output results are distributed spatially and temporally.
Disadvantages ⊖	
Not representative of a heterogeneous medium	Greater calculation times
Not able to represent multiple contamination sources	Numerous input parameters were requested
Not able to represent irregularities given by the geometric conformation of the site and by the contamination source	Numerical instability problems that can make the mathematical resolution of the system more complicated
Not able to represent temporal variability of physical phenomena	

3.4.2. 3D Modelling for unsaturated soils

A phreatic aquifer is replenished from above by water from various sources: precipitation, irrigation, artificial recharge by surface spreading techniques, etc. In all these cases, water moves downward, from the ground surface to the water table, through the unsaturated zone. The understanding of, and consequently, the ability to calculate and predict the movement of water in the unsaturated zone is, therefore, essential when we wish to determine the replenishment of a phreatic aquifer.

A second example is related to groundwater contamination from sources at the ground surface. Contaminants from such sources dissolve in water applied to the ground surface. The infiltrating water will then carry the dissolved contaminants as it moves downward towards the water table. Various phenomena, e.g., dispersion and adsorption, occur as contaminants travel downward with the infiltrating water. These affect the concentration of pollutants in the water, eventually reaching the water table. The ability to forecast the movement and accumulation of contaminants in the unsaturated zone is required to clean the subsurface from these contaminants or to determine the rate at which they will reach the water table. However, one cannot study the movement of contaminants carried by the water without information on the movement of the water itself [8].

Once the conceptual model has been defined, it will be possible to proceed to the development of 3D modelling for unsaturated soils with the scope of:

- Support the definition of the conceptual model of the site.
- Identify the presence or absence of contamination.
- Verify the respect of the threshold limits in the unsaturated soil.
- Quantify impacted soil volumes.

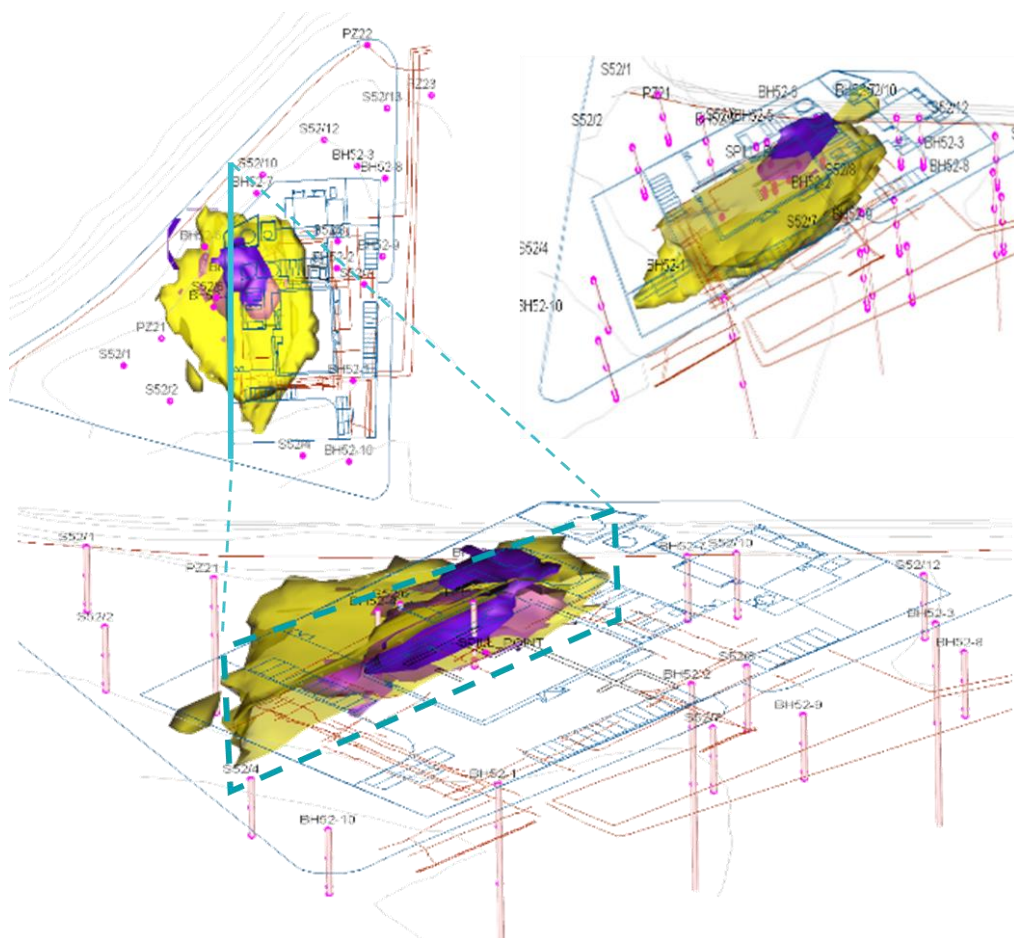


Figure 5: Example of a three-dimensional representation of the presence of contaminants.

Contamination should be defined regarding source and substance if contamination is detected. The following steps should be followed to characterise soil pollution:

- Identify the possible source of contamination.
- Define the concentration of pollutants for each borehole, classifying the sample depth (superficial, intermediate, and deep).
- Identify intervention and investigation concentration levels for the substances.

Using appropriate modelling software, interpolation algorithms can be applied to obtain the 3D spatial distribution of the contamination detected in the soils. The volume of soil excavated and disposed of can also be evaluated.

3.4.3. 3D Modelling for saturated soils and groundwater

The scopes of 3D Modelling for saturated soils and groundwater can be summarised as follows:

- Numerically support the definition of the Site Conceptual Model.
- Be a technical tool for understanding the hydrogeological system under examination.
- Define the presence or absence of contamination and any containment actions.

A numerical model should be used to apply this methodology, more suitable for the analysis of complex hydrogeological systems [9]. Such models allow us to study systems in which are present:

- Multilayer aquifers.
- Changes in the hydrogeological parameters of the aquifer, such as hydraulic conductivity.
- Changes in the thickness of the aquifer.
- Water inputs/outflows outside the system.

The 3D modelling can be carried out following these sequential phases:

1. Model construction: providing the main input data used to construct the model.
2. Model calibration and validation: carrying out the calibration procedure adopted (residue analysis) and the verifications on the model.
3. Transport model: describing the phenomena influencing the compounds' transport and identifying sources and concentrations of the Compounds of Concern.
4. Transport simulation: providing results obtained from simulations of the substances transport along with the groundwater flux over the model area.

To complete the 3D modelling, the flow model should be defined, which means that:

- The model domain is defined, and its horizontal and vertical discretisation is carried out.
- The geometry of the hydrogeological system and the hydrodynamic parameters are defined.
- Boundary and initial conditions are implemented.
- The numerical groundwater flow model is validated.
- The model transport is implemented.

The term “flow equation” indicates a mass balance equation for a fluid phase combined with the appropriate form of Darcy’s law (motion equation) [10]. The objective is to obtain a single equation for that phase, written in terms of a single state variable, such as pressure or piezometric head [11]. In the case under evaluation, we shall use the mass balance equation for a three-dimensional saturated flow of water. The transport model verifies the spatial distribution of the compounds of interest within the area of interest.

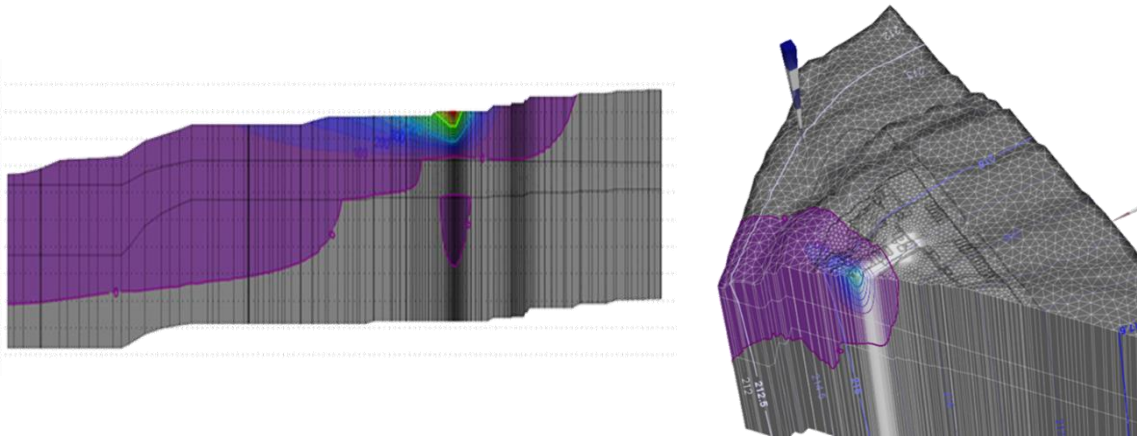


Figure 6: Example of the output of 3D groundwater modelling, showing the presence of a plume of contamination.

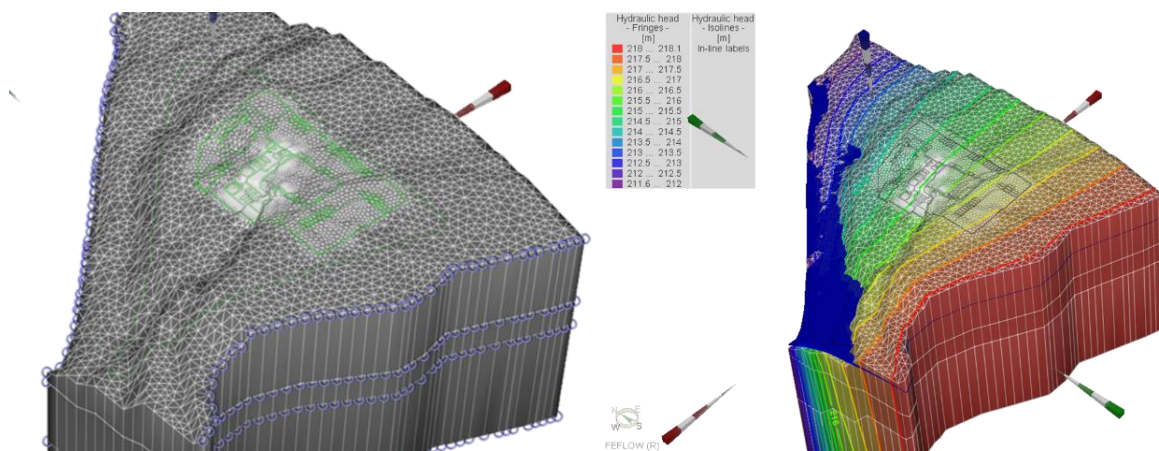


Figure 7: Example of the representation of 3D groundwater modelling domain and parameters.

The term ‘transport’ is intended as ‘movement, storage, and transformations’, with the term ‘transformations’ indicating changes in concentrations of dissolved chemical species as consequences of chemical reactions and interphase transfers, such as dissolution of the solid matrix and precipitation [12]. The transported quantity is the mass of the fluid phase. In contrast, in a contaminant transport model, the transported quantity is the mass of the chemical species - the contaminant - carried by that phase. In the first case, the intensive quantity is the fluid mass density, while in the latter case, it is the concentration of the chemical species. Furthermore, we may have to consider simultaneously several interacting chemical species [7]. The transport of pollutants that can occur can be modelled in different ways. The different types of pollutant transport are listed below:

- Physical, including:
 - Advection refers to the bulk movement of solutes carried by flowing groundwater.
 - Dispersion refers to the spreading of the contaminant plume from highly concentrated areas to less concentrated areas. Dispersion coefficients are calculated as the sum of molecular diffusion, mechanical dispersion, and macro-dispersion (see Figure 8).
 - Diffusion is the process by which a contaminant in water will move from an area of greater concentration toward an area where it is less concentrated (see Figure 8).
- Reaction, adsorption and decay rate: this category includes all the elements attributable to decay, transformation, biodegradation, adsorption, and delay reactions related to the physical characteristics of the materials considered.
- Chemical, including precipitation/solution, chemical reactions, and adsorption/ desorption.

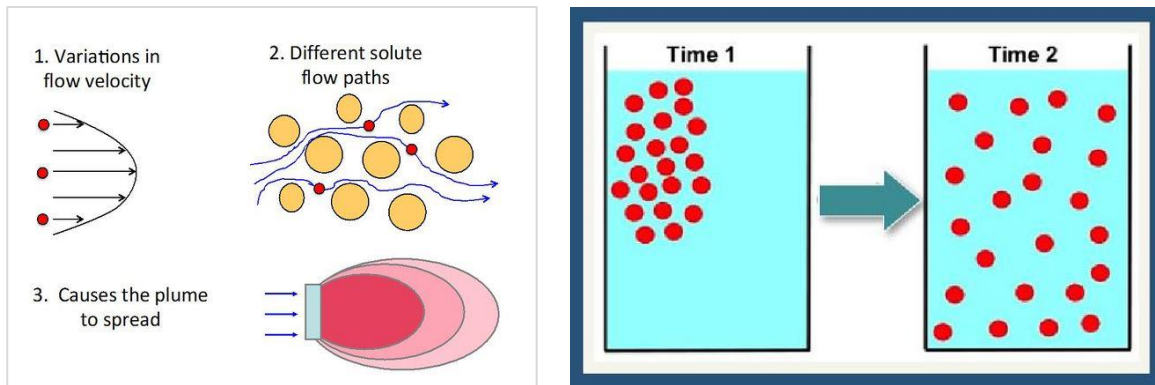


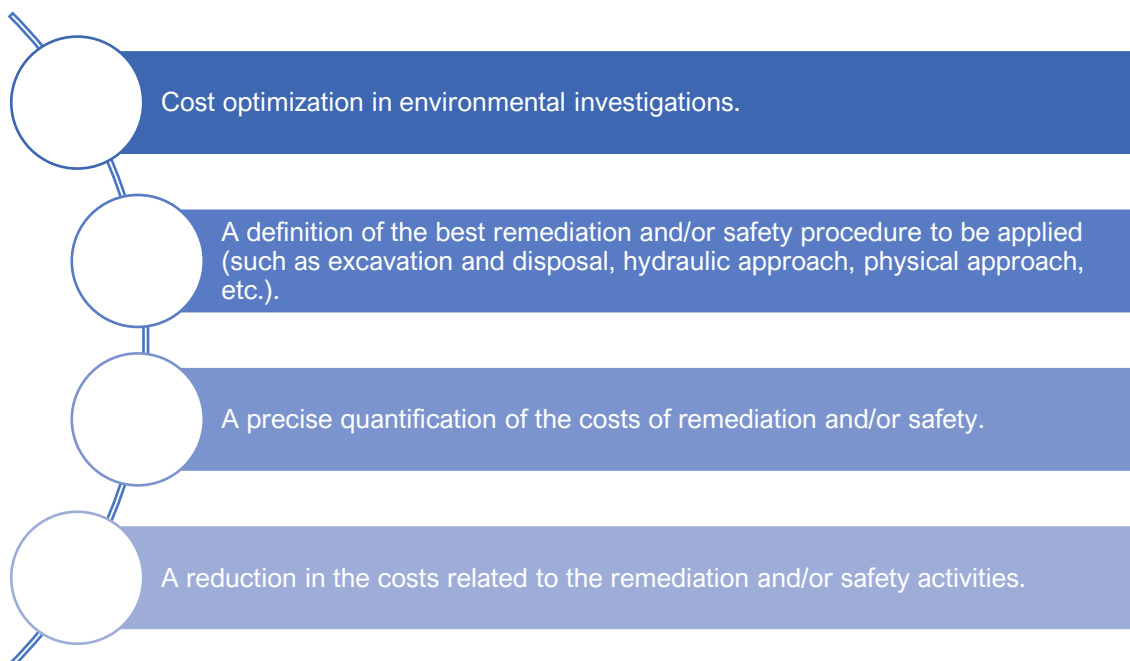
Figure 8: Schematic representation of mechanical dispersion (on the left) and diffusion of a dissolved chemical recently placed in a container at Time 1 and then distributed throughout the container at Time 2 = Time 1 + Δt (on the right). [13] [14]

4. CONCLUSIONS

The results obtained by following the methodology described allow us to quantify the impacted portion of soil and aquifer to define the best management techniques and remediate the study area. The methodological approach developed within this document allows to:

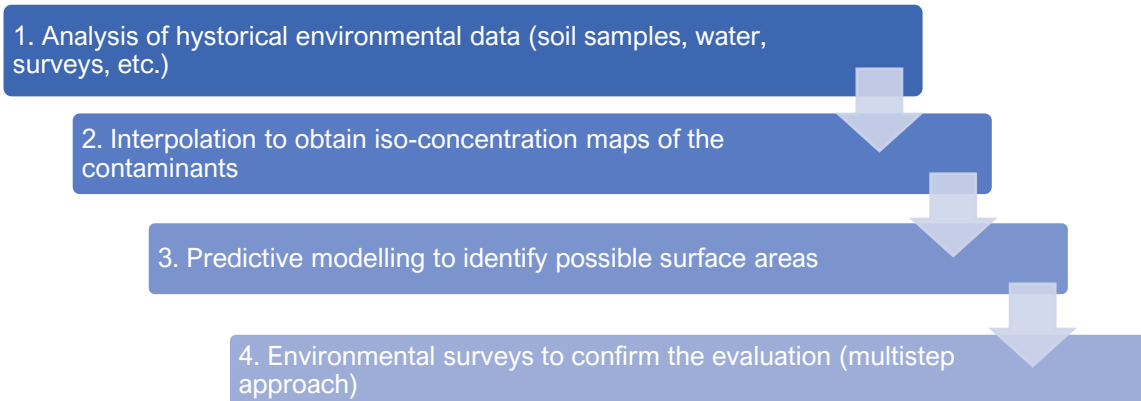
- Define the state of environmental characterisation of the area of interest to highlight the areas where environmental data have been found poor/unsatisfactory.
- Prepare a specific environmental investigation plan for distributing the information for the study area.
- Identify and delimit the potential source of contamination.
- Delimit contaminated unsaturated soils with good approximation and quantify impacted volumes.
- Delimit the portion of the contaminated aquifer.

The results obtained are fundamental in the process of managing the contamination and remediating the area of interest, allowing:



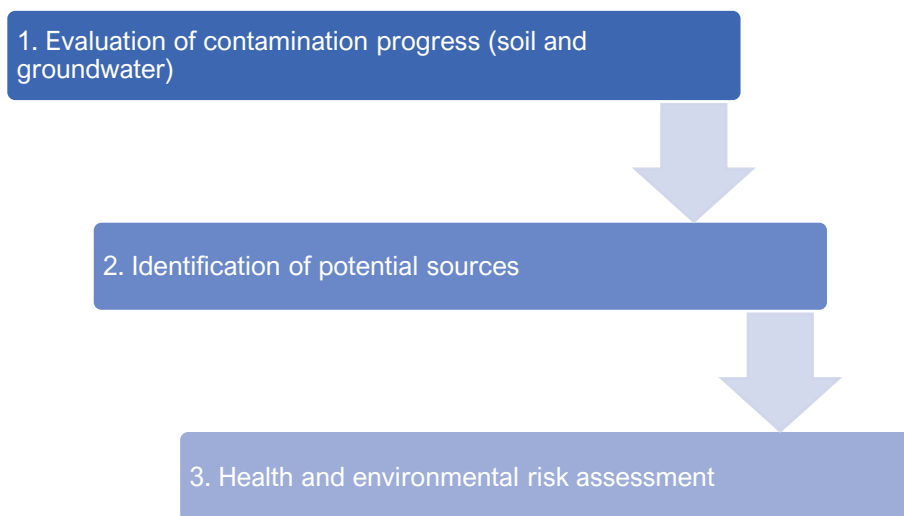
As regards the possible future developments of the methodology, two possible scenarios identified are described below:

Identification of potential sources by analysis of historical and current data, following these steps:



The innovation introduced with this type of modelling is predictive models, used to predict future events or outcomes by analysing patterns in each input data set.

Identification of intervention priorities and best approaches, following these steps:



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