Hydrogeological processes and geological settings over Europe controlling dissolved geogenic and anthropogenic elements in groundwater of relevance to human health and the status of dependent ecosystem

Deliverable 8.2.

RECOMMENDATIONS FOR MONITORING OF KEY PARAMETERS WITH REFERENCE TO ENVIRONMENTAL CONTEXT, GEOLOGICAL SETTING AND RISK ASSESSMENT

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GENERAL INTRODUCTION

As reported by Norman network (https://www.norman-network.net/), emerging substances can be defined as compounds that have been detected in the environment, but which are currently not included in regular monitoring programmes at EU level. Many Contaminants of Emerging Concern (CECs), are classified as pseudo-persistent compounds (Torres-Padrón et al., 2020), due to the fact that they are continuously released, putting the focus on modes of entry into the environment rather than taking into consideration an intrinsic property of the substance.

The criteria under "Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals" (REACH) to classify a substance as persistent is its half-life for biodegradation to be more than 60 days in water and more than 180 days in sediment or soil. In the context of this legislation, the German Authorities proposed in 2017 criteria for the identification of persistent chemicals that are mobile in the aquatic environment. Substances meeting these criteria are known as persistent, mobile and toxic (PMT) or very persistent and very mobile (vPvB) (Neumann et al., 2015; Neumann, 2017; Neumann and Schliebner, 2017a, b).

Human activities resulting in discharge of CECs to surface water have been the focus of numerous investigations, aiming to analyse its impact on streams, lakes, terrestrial dependent ecosystems and coastal waters. The first Watch List for emerging water pollutants (Carvalho et al., 2015), published in mid-2015 (Commission implementing decision, 2015. No longer in force, Date of end of validity: 05/06/2018; Repealed by 32018D0840), focused on surface waters and it aimed to provide information on the concentration of substances of potential concern in the aquatic environment.

The presence of CECs in groundwater has been analysed for both targeted studies and broad reconnaissance surveys (Lapworth et al., 2012, Bunting et al., 2020). According to the authors, groundwater occurrence is poorly characterised and understanding temporal and spatial variation remains a priority. In order to address the problem, sampling campaigns have been carried out in Europe. Although most of them were at a regional scale (Bunting et al., 2021), as an example, in the work from Lopez et al. (2015), a nationwide screening of 411 emerging contaminants was done at 494 groundwater sites throughout France. Kivits et al (2019) took into account the environmental setting and groundwater age in consideration when studying veterinairy antibiotics.

It follows that there is a need to include into the monitoring programmes these types of currently unregulated substances that may have influenced groundwater for a more sustainable water policy. The technical Group on Groundwater (GIS GWW) was mandated by the European Commission to elaborate a concept for the elaboration of a Groundwater Watch List to facilitate the identification of substances for which groundwater quality standards or threshold values should be set (Lapworth et al., 2019).

The objective of this report is to inventory approaches that help to assess and predict concentration of CECs in groundwater, to estimate the limits for their application and review relationships between the occurrence of emerging organic contaminants in groundwater and environmental settings. For instance, concentration of CECs in groundwater has been correlated to soil condition, hydrological parameters and hydro-climatic conditions and residence time indicators. Analytical limitations and the possible use of statistical methods to evaluate the results are also presented.

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1 APPROACHES TO CORRELATE CONCENTRATION OF CECS IN GROUNDWATER

Depending on data availability, the contaminants involved, the environment and the objectives pursued with the study, several different approaches may be found to link concentration of CECs in groundwater with other external drivers. They vary from qualitative insight into patterns of distribution to complex statistical methods to identify and analyse all factors that could have an impact on groundwater concentration.

1.1 Overlay methods

Overlay analysis is the simplest form of spatial modelling (Jerrett et al., 2010) and is based on overlapping different layers of environmental characteristics. The superposition of GIS layers with selected parameters (like the depth of the unsaturated zone) allows comparison of the influence of several parameters on the generated maps.
Visual representation of data clearly communicates insights from data and information, showing associations between detection or concentration data and possible correlation with geological setting, land use or hydrogeological features.
In some cases, there is a positive correlation between concentration in different environmental matrices and, in others, concentration in sediments is greater than that in water, pointing out the trend of some compounds to accumulate in sediments.
In Switzerland, the Federal Office for the Environment FOEN (2019) superimposed data at national level regarding aquifer type (consolidated or unconsolidated), percentage of wastewater in water courses, type of monitoring station (extraction well, piezometer and spring) and perfluorinated chemicals concentration (PFC) in groundwater. They concluded, based upon that information, that infiltration of surface water with treated or untreated wastewater into groundwater appear to be the major source of PFC in Swiss groundwater. Moreover, most PFC detections were made at unconsolidated aquifers.

1.2 Index vulnerability methods

The estimation of groundwater vulnerability is essential to analyse the facility with which groundwater can be contaminated by human activities. The Minnesota Department of Natural Resources (Minessota DNR, 2016) defines an area as sensitive if natural geologic factors create a significant risk of groundwater degradation through the migration of waterborne contaminants. Vulnerability is generally calculated by the combination of the intrinsic vulnerability with an indicator or proxy (European Commission, 2018) of the emerging contaminant of concern (or family).
In the report of Broda et al. (2019), some 50 methods to assess groundwater vulnerability were identified, from rating systems to mathematical models or multi-criteria analysis. The authors compare commonly applied index methodologies in Europe to assess the vulnerability of the upper aquifer.

Yet, there are substantial uncertainties in all approaches to vulnerability assessment. Index methods, for instance, are based upon an assumption of a generic contaminant, and different climatic conditions or aquifer types require different approaches.
Often, several methods are implemented (Thapa et al., 2018) to select the most appropriate one in predicting vulnerable zones. The result is a set of qualitative risk categories, linked to aquifer vulnerability.

1.3 Statistical models

While overlay methods deals with visualization techniques, there is a wide array of statistical models to study the behaviour of CECs in groundwater, from single qualitative studies to complex quantitative analysis with more than one variable involved. Often, more than one statistical technique can be applied to account for their occurrence and distribution.
In some cases, it is of interest to assess the degree of association of two quantitative variables, either because there is not enough data to perform a multivariate analysis, or because it is interesting to analyse the influence of a single variable in pollutant concentration in groundwater.
One of the most powerful tools to draw conclusions consists in analysing the relationship between at least two variables by means of correlations. This technique of information analysis provides the strength and sense of the relationship.
For example, levels of insecticides in soil (Aznar-Roca, 2016) were analysed by means of Spearman correlation test, while Wilcoxon rank sum analysis was used to analyse the influence of primary land use around the wells (300 buffer area) on concentration of surface derived contaminants (IDGR, 2015). In the same study, Spearman's rank correlation tests between groundwater-quality parameters and concentration and/or numbers of CECs. García-Gil et al. (2018) found significant correlation between UV-filters, antibiotics and total CECs contents and pH through the same correlation coefficient.

1.4 Numerical simulation models

Groundwater flow and transport processes can be assessed by means of numerical simulation models. While numerical simulation is a cost-effective approach to study complex systems, a number of simplifications and assumptions are necessary. The implementation of the outcomes of models designed for use in porous media in karst terrains is a common limitation.
On the other hand, occurrence of CECs in groundwater is relatively recent, and current knowledge on this subject area is scarce. In recent times, numerical models have been applied to simulate spatial distribution of parameters, like groundwater age (Toews et al., 2016).
Most numerical models of groundwater flow and reactive transport of pollutants consider solid-phase sorption as the only retardation factor. However, additional processes may affect transport of certain pollutants in source areas. For example, considering that many PFAS are surfactants, adsorption at the air-water interface in the unsaturated zone, NAPL-water partitioning and NAPL-water interfacial adsorption are factors likely to influence (Brusseau et al, 2019) transport and retardation.

In the work of García-Gil et al (2018), the exploitation of shallow geothermal resources in the urban aquifer of Zaragoza (Spain) is found to be a significant element controlling the degradation of organic pollutants (mainly antibiotics and UV filters). In such settings is then necessary to include this factor in the numerical fate and transport model.

In HOVER WP5 tracer-based infiltration year patterns with model-based infiltration year patterns were compared in a pilot study. For this purpose, they applied the National Hydrological Model of the Netherlands to determine groundwater ages for each of the observation wells that were used in the tracer study, applying a particle tracking approach using MODPATH and a single solute transport approach using MT3DMS. Although the modelled patterns resemble the tracer patterns for the solutes and pesticides studied, it was observed that the spatial resolution of the model did not allow for a proper age determination of part of the wells, generally leading to an overestimation of the groundwater age in part of the wells. As a result, modelled pesticide hits and elevated nitrate concentrations were unjustly linked to infiltration periods before 1970 (HOVER D5.3)

2 SCALE OF INVESTIGATION

Many studies have proved a significant impact on local groundwater sources (García-Gil et al., 2018; Hu et al., 2016; Corada-Fernández et al., 2015; Estévez et al., 2012). In response, targeted studies have been frequently carried out at aquifers near pollution sources, where high concentrations of different kinds of CECs have been found. In such studies, correlation between their concentrations and single factors related to environmental settings suggests that there might be other elements affecting CECs concentration and distribution.

On the other hand, broad reconnaissance studies have been carried out to assess distribution of CECs through groundwater bodies (Montesdeoca-Esponda et al., 2021), catchments (Llamas et al., 2020; Karpuzcu et al., 2014) or even countries (Lapworth et al., 2018; Manamsa et al., 2016; Lopez et al., 2015).

In some cases there is spatial continuity, which means that a significant spatio-temporal dynamics can affect distribution of substances of concern (*Table 1*).

Method	Targeted	Reconnaissance studies	
		Spatial continuity	Discontinuity
Overlay methods		*	*
Index vulnerability methods		*	
Statistical models	*	*	*
Numerical simulation models		*	

Table 1: Relationship between methods to study emerging contaminants and scale of investigation

3 CONCEPTUAL MODEL

A conceptual site model (CSM) is essential to understand fate and transport of (emerging) contaminants in the physical environment. Natural systems are very complex and all conceptual models are by definition only a simplified or partial representation of natural physical processes. Models are used to present a simplified representation of some real world phenomena (Fetter, 2001).

Conceptual models do not have necessarily to be numeric (European Commission, 2009), but must reflect the geological and hydrogeological features of the analysed system.

Aquifer conceptualization provides knowledge for an effective groundwater management and corroborates that the analytical results come from the same groundwater body (GWB) or hydrostratigraphic unit (*Figure 1*).

If there is a lack of understanding of the groundwater flow system, the analysis of concentration data from monitoring networks will provide erroneous conclusions about what processes are occurring within the groundwater body. But when the sources of contaminants are well known on a specific groundwater catchment area, it is possible to use monitoring results to increase the understanding of transfer pathways. For example, Lamastra et al. (2016) propose the use of carbamazepine, galaxolide and sulfamethozale as environmental tracers to improve the elaboration of the CSM.

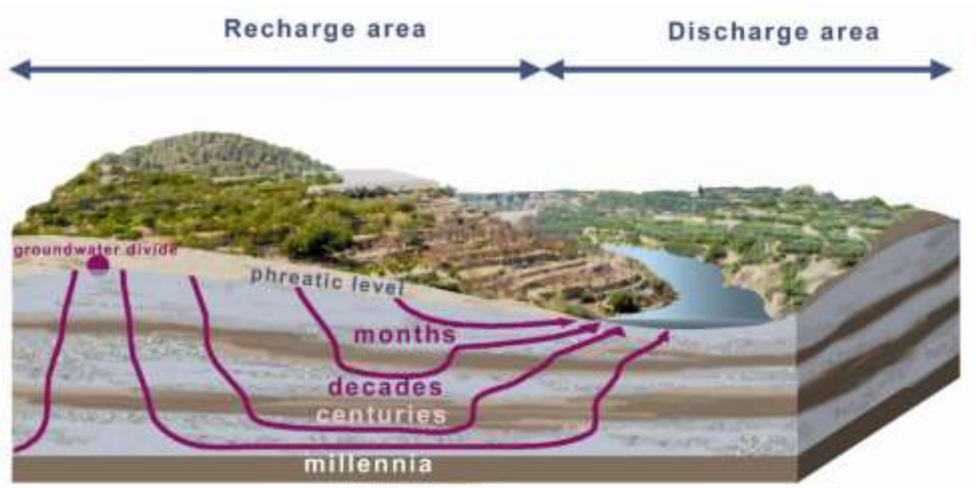

Figure 1: Recharge and discharge areas, flow lines and residence time of water in an aquifer, from López-Geta et al., 2006)

4 ENVIRONMENTAL FACTORS AFFECTING CECS PRESENCE IN GROUNDWATER

Fate and transport of emerging contaminants and their transformation products in the aquatic ecosystem depend on several factors, among others, input sources, structural properties, geological, hydrogeological and environmental settings.

Occurrence of CECs in groundwater is not a random variable, but due to a combination of natural and anthropogenic factors, which can be split into several categories (Table 2).

4.1 Primary factors

The primary factors affecting distribution of CECS in groundwater are soil properties, geological setting, aquifer and groundwater properties and hydrological processes.

	Potential drivers	Properties	Main influenced process
Primary factors	Soil properties	• Organic carbon content • pH • Clay content • T°	• Mobility (Adsorption) • Biodegradation • Transformation products
	Geological setting	• Lithology • Permeability	• Mobility (Adsorption)
	Aquifer and groundwater properties	• Unsaturated zone thickness • Hydraulic conductivity • Groundwater age • pH • redox conditions • Dissolved oxygen	• Speed of transfer • Dilution
	Hydrological processes	• Relationship river-aquifer • Climate • Flow condition • Seasonal variation	• Distribution of CECs
	Land use	• Actual/historical land use	• Type of contaminants • Distribution of CECs

	Potential drivers	Properties	Main influenced process
Additional drivers	Extent of pollution	• Spatial character • Distance to source	• Concentrations • Distribution of CECs
	Groundwater well characteristics	• Depth • Pumping rate • Age	• Distribution of CECs • Travel time
Features of prevalent contaminant	Physico-chemical properties	• Water solubility • Acid dissociation constant • Structure and size • Hydrophobic interaction	• Distribution of CECs
Source area processes	Interaction with other contaminants	• Synergistic effects • NAPL-water partitioning and NAPL-water interfacial adsorption	• Transformation/combined products

Table 2: Factors influencing the occurrence of CECs in groundwater

4.1.1 Soil properties

Soil properties can affect attenuation processes as contaminants move through the unsaturated zone. According to some studies (Li and Kookana, 2018), organic carbon content, pH and clay content are required to predict the way the contaminant will behave in soil.
Processes of biodegradation can also occur in soil, depending on microbiological communities and their activity driven by some parameters like temperature, humidity…

4.1.2 Geological setting

Geology is one of the major driving forces controlling groundwater flow. Permeability of the sediment is the controlling factor that contributes to the vulnerability. The starting point for groundwater modelling is often the assumption of uniform, ideal porous media. However, even homogeneous formations are non-uniform, and subsurface heterogeneity influences groundwater dynamics.

Some others, like karst aquifers, exhibit a highly anisotropic character with preferential flow pathways. Lack of correlation between groundwater concentration, source and depths, indicates the existence of preferential flows in fractured materials (Estévez et al., 2012).

4.1.3 Aquifer and groundwater properties

Vulnerability of aquifers to pollution depends on their hydraulic properties. It seems reasonable that detection frequencies of emerging contaminants are greater in unconfined aquifers that in confined ones because of a greater intrinsic vulnerability to surface land use.

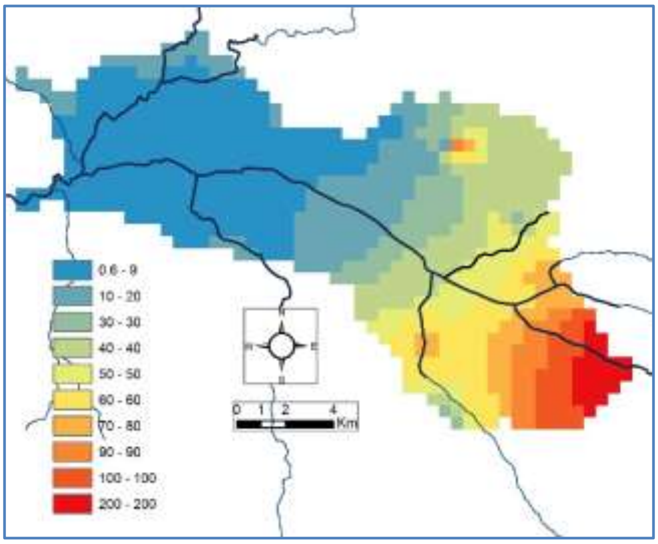

Figure 2: Estimation of unsaturated zone thickness in Vega de Granada aquifer

Unsaturated zone thickness

The unsaturated or vadose zone controls migration of water and pollutants and transformation mechanisms of the latter. The functioning of this zone is very complex, due to its chemical, biological and microbiological interactions. This complexity of relations within the unsaturated zone requires modelling approaches (*Figure 2*).
In the study of (Høisæter et al., 2019) unsatutared column studies were performed, showing that PFOS is strongly attenuated in the unsaturated zone.

Age

Knowledge of the relative age of groundwater and its distribution can help determine whether groundwater is vulnerable to surface-related contamination (Iowa DNR, 2015) and it is a valuable input to the development of the conceptual model (e.g. Lapworth et al., 2006 ; 2018).

It also help to determine the vulnerablity to diffuse sources. See for example Kivits et al. (2019) or Visser et al. (2009).

pH

Groundwater physico-chemical properties are a key factor in the fate and transport of CECs. Garcia-Gil et al. (2018) provide evidence regarding dependency of mobility of UV-filters and Personal Care Products (PCPs) in groundwater with pH.

Redox conditions

Redox conditions, which affect the persistence of some contaminants (i.e. younger groundwaters are more likely to be fully saturated with respect to dissolved oxygen. Oxic conditions are found in surficial groundwater bodies composed of unconsolidated sediments or crystalline rocks.
In the latter, rapid migration of groundwater through fractures can occur (Bexfield et al., 2019).

Dissolved oxygen

Erickson et al.(2014) related higher dissolved oxygen concentrations to shorter duration flow paths from the land surface.

4.1.4 Hydrological processes

While most groundwater comes from meteoric water, in the form of rain or snow, surface run-off is, to a smaller extent, an important source of groundwater recharge, as surface water and groundwater systems are usually connected (*Figure 3*).
Climate and flow conditions are related to the availability of water resources and may affect flow direction substantially. Moreover, in certain aquifers, such as karstic ones, recharge from surface water can be the driving force that determines groundwater concentrations in pollutants.
In summary, groundwater and surface water are interconnected resources, so spatial and temporal variations of flow rate in rivers, for instance, can play a major role in the type and concentration of compounds detected (Manamsa et al., 2016).

Relationship river-aquifer

Surface-groundwater interactions provide a link between surface water (rivers, lakes and wetlands) and groundwater and it is based on the existence of water exchange pathways between groundwater and surface water courses that run on or near to permeable formations (Ballesteros et al., 2019). Changes in groundwater levels, for example, may cause an inversion in flow direction.
Depending on the origin of groundwater recharge, a different pollution transport mechanism and, consequently, concentration, is predictable using a source-pathway-receptor framework.

It is foreseeable that aquifers recharged directly by surface water will respond differently to pollution in river than that of confined aquifers.
In the same way, groundwater can discharge into surface water bodies. Its implications include the transport of emerging contaminants. Urban sprawl implies not only land use changes, but also the creation of impervious surfaces.

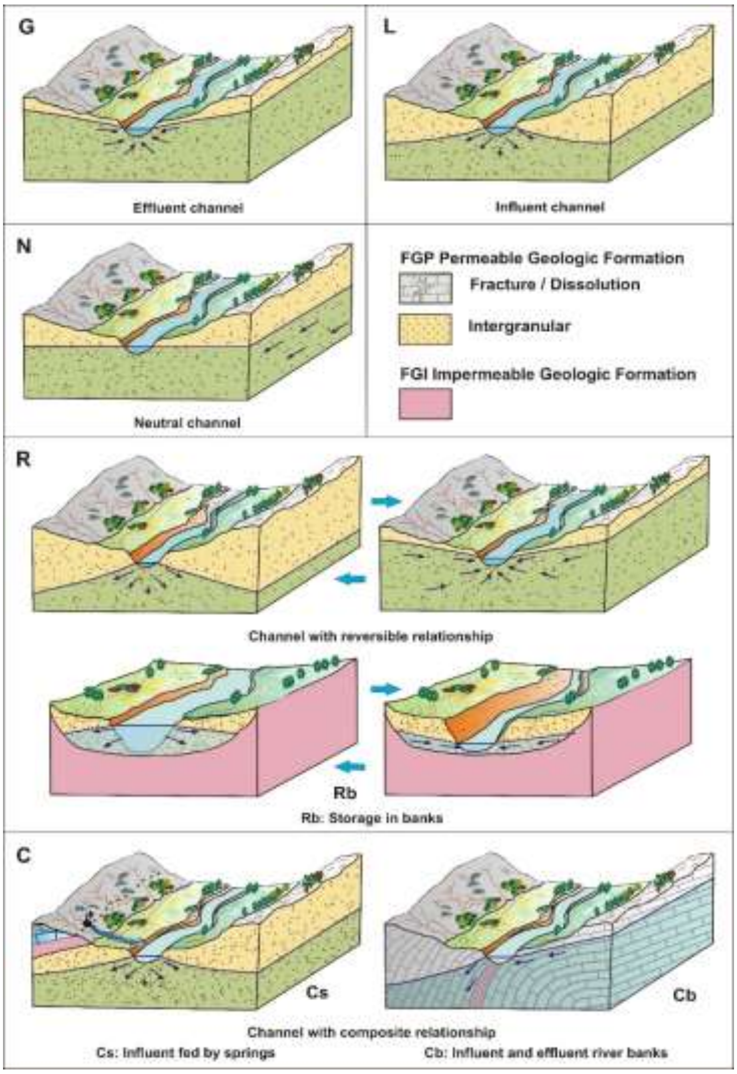

Figure 3: Classification of river groundwater interactions based on water direction (modified from Ballesteros et al., 2019)

As a result, a multitude of urban pollutants are discharged into the streams without treatment. Sustainable Urban Drainage Systems (SUDS) are designed to decrease run-off and associated pollution. SUDS explicitly enhance urban groundwater recharge often with little or no enhanced

pollution attenuation - or may enhance bypass of natural attenuation mechanisms in the soil. In summary, this separation between surface water and groundwater is artificial.
However, their interactions have often been overlooked when studying fate of emerging contaminants in different environmental matrices and compartments (Manamsa et al., 2016).
In fact, although in many watersheds, surface water features are hydraulically connected to groundwater, their interactions can be difficult to quantify (Ballesteros et al., 2019). Depending on the regional flow component, the authors classify river aquifer systems (*Figure 3)* according to water direction. It describes whether the water exchange is in favor of surface runoff (predominant underflow component), or to aquifers (predominant baseflow component) or mixed. Such relationship must be clearly identified when delineating the conceptual model

Climate

The rainfall regime controls the availability of water. As mentioned by Lang et al. (2017), rainfall can induce modifications in release rate and therefore groundwater concentration. Recharge under different climate conditions is highly variable. In arid and semi-arid regions, with high evaporation rates, the reuse of treated wastewater for crop production (or other types of water reuse in densely populated areas) is a common practice. Zemann et al. (2016) showed an increase in the potential for evaporative accumulation of bezafibrate and carbamazepine under simulated arid conditions. Sorensen et al. (2015) showed a seasonal change in DEET concentrations in groundwater.
On the other hand, climate change will increase the risk of flooding, which results in different impacts on groundwater. For instance, groundwater chemistry is affected by concentration, which may vary, in turn, after flooding. In addition, the above causes of groundwater impacts are often inter-linked, and it can be challenging to isolate the effects of each of them.

Flow condition

Very variable flow regimes can alter hydraulic conductivity of riverbed sediments, by erosion or deposition, and thus affect intensity and direction of exchange. Spatial distribution of the underground flow system also influences intensity of natural groundwater discharge. Munoz et al. (2016) associate low-flow conditions to PFAS concentration peaks in river Seine, while Kibuye et al. (2019) found that the mean concentrations detected in groundwater samples were generally higher than concentrations in surface water samples, attributing a dilution effect to high-flow conditions in surface water.

Seasonal variation

Numerous studies have shown that CECs concentration in shallow groundwater bodies, while depends upon the geological setting and type and source of contaminant, it often varies with recent recharge conditions (Iowa DNR, 2015). Bai et al. (2018) analyse pharmaceutical and waste indicator compounds and pesticides in surface waters. CECs concentrations were correlated to streamflow volume and showed significant seasonal effects. Hence, if the conceptual model shows interactions of groundwater with a river, seasonal effects should be investigated.

4.2 Additional drivers

A numer of factors are likely to play a major role in influencing primary drivers, as well as other indirect drivers.

4.2.1 Land use

A number of studies have been carried out to determine whether concentration of contaminants in groundwater can be associated to nearby land use use (Lapworth et al. 2015; Snow et al., 2017; Bexfield et al., 2019). In a study of the contents of pharmaceuticals and hormones in ground-water taken from the national groundwater monitoring network in Poland, Kuczyńska (2019) found variations in the distribution of pharmaceuticals depending on land use type.
Other studies, through the evaluation of public well vulnerability classification for contaminants of emerging concern (IDGR, 2015), found no significant correlation due to low detection frequencies, but median and maximum atrazine concentrations were lower in wells located in row crops.
According to Estévez et al. (2012) irrigation with reclaimed water is especially significant in arid areas and it is likely to increase the amount of emerging contaminants entering the aquifer.

In *Figure 4* land uses of Vega de Granada aquifer and probability of caffeine detection by means of kriging indicator is showed. Irrigation crops and urban areas exhibit the higest concentration values (marked in red in the figure on the right).

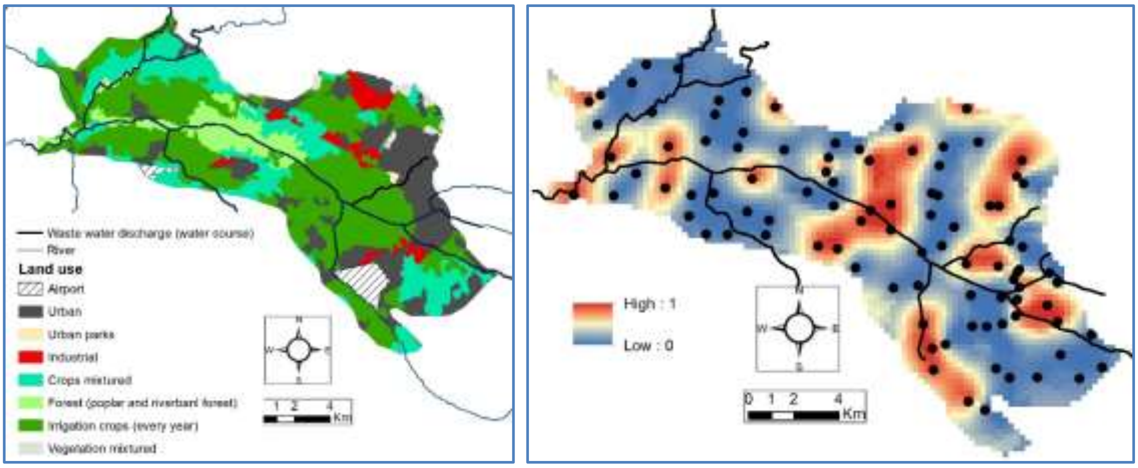

Figure 4: Probability of caffeine detection by means of indicator kriging

Snow et al. (2017) analysed 79 papers published in 2016 and provides a detailed description of occurrence and fate of emerging contaminants likely to occur in agricultural soils. One of the reviewed papers (Fairbairn et al., 2016) provides evidence of a correlation of concentrations and loadings to land use and flow conditions.

4.2.2 Extent of pollution

Sources of CECs can be broadly classified in two types (*Table 3*): point and diffuse sources. While agriculture is considered one of the prevailing diffuse sources, industrial and urban areas, usually considered as point source pollutions, are responsible for the introduction of a number of emerging contaminants into the environment. Atmospheric transmission of CECs is also an important pathway for diffuse and possibly wide-spread contamination of the natural environment.

The main pathway of introduction into groundwater bodies is infiltration and polluted residual waters. While point source pollution originates from discrete locations and is of limited spatial extent, diffuse sources are limited to large areas and can cause larger impact on groundwater quality. Sometimes, point sources may originate diffuse pollution, as it is the example of agricultural land irrigated with treated effluent.

Point sources are associated to many anthropogenic activities, among which the most significant are those accomplished in wastewater treatment plants, fire training areas, industrial sites and airports. In addition to point sources, a number of activities that have no specific point of discharge may be potentially responsible for the introduction of CECs into the aquifer.

4.2.3 Groundwater well characteristics

There are several factors to consider when analysing data from monitoring networks. In terms of pollution vulnerability, it is evident that the depth of a well is linked to travel time of contaminants.

In the course of a comprehensive study of contaminants of emerging concern in Iowas' groundwater (IDGR, 2015) well age, well depth and pumping rates were correlated with concentration of contaminants. While more recently drilled wells had lower concentrations of atrazine, higher pumping rates were significantly positively correlate to acetanilide degradates.

	Point Sources	**Diffuse sources**
Urban	Urban waste stream Buried septic tanks	Storm-water and urban runoff Leakage from reticulated urban sewerage systems Sewer overflows Diffuse aerial deposition Illicit discharges
Industrial	Manufacturing plants Hospitals Food processing plants Industrial impoundments Resource extraction Fracking chemicals	Diffuse aerial deposition Illicit discharges
Agricultural	Farm wastes lagoons	Livestock and poultry Agricultural runoff from bio-solids and manure sources Application of pesticides (Legacy or modern) Diffuse aerial deposition

Table 3: Summary of input sources of emerging contaminants. Emerging contaminants can reach groundwater bodies via different sources and pathways.

From the risk assessment perspective, the classical approach source-pathway-receptor has been used to understand the entrance of emerging contaminants into groundwater bodies.
In the study of Heberer et al. (2004), several pharmaceutically active compounds (PhACs) were found in groundwater samples from bank filtration sites, such as carbamazepine and especially primidone.

Distance to source

In the work of Qian et al. (2015), high concentrations of caffeine and paraxanthine were measured in a septic tank. Concentrations were decreasing with distance to source and depth in groundwater, downgradient of the source.

4.3 Features of prevalent contaminant

4.3.1 Physico-chemical properties

Emerging contaminants comprise thousands of individual compounds (Montagner et al., 2019). The chemical properties of a substance determine its behaviour in environmental media and interaction between substances has a complex effect on adsorption. There are wide differences among families with different physical-chemical properties (Llamas et al., 2020) even inside the same type of compound, so caution must be applied when analysing their behaviour.
A large number of chemicals are potentially present in the aquatic environment, and their properties influence their fate and transport in the unsaturated zone. Kibuye et al. (2019) found that extent of groundwater contamination by pharmaceutical compounds is controlled by both compound sorption potential and biodegradability.

4.3.2 Water solubility

The polarity of a compound determines its mobility in the aquatic environment. Hydrophilic molecules have high polarity (low log Kow values) and thus higher solubility. Therefore, they may end up in groundwater, in contrast to less mobile hydrophobic compounds, with higher degree of interaction with soil materials (Del Rosario et al., 2014).
Some compounds, like certain flame retardants have low solubility in water, so they tend to sorb to sediments in rivers, while some organic solvents, like MTBE and ETBE (Reemtsma et al., 2016) have high solubility and poor biodegradability and are, therefore, more frequently detected in groundwater.

4.3.3 Acid dissociation constant

The degree of ionization of a substance depends on its acid dissociation constant (pKa), which is affected by the pH of the water (Lapworth et al., 2012). Vierke et al. (2013) shows that pH of water and pKa are the key factors in the extent of volatilization of PFCAs in the environment.

4.3.4 Structure and size

Partition into aqueous phase depends on chain length in some cases. To cite an instance, PFAS with fewer than eight carbons are more likely to partition to aqueous phase (Huset et al., 2011) and branched isomers have less sorption than linear (Kärrman et al., 2011).

4.3.5 Hydrophobic interaction

The influence of different substances on sorption, like oil and other organics, has been investigated in the work of Sepulvado et al. (2011), discovering that they may increase sorption. In another study, Barzen-Hanson et al. (2017) also found that sorption of some types of PFAS (FtSaBs and FtSaAm) was driven by hydrophobic interactions.

4.4 Source area processes

Often, emerging contaminants occur as mixtures in the environment. Little is known about synergistic and antagonistic actions of these compounds in groundwater. In the study of Brusseau et al. (2019) retardation of PFAS in the presence of NAPL is analysed, and evidence of influence of NAPL-water interfacial adsorption is provided.

5 OCCURRENCE OF EMERGING CONTAMINANTS IN GROUNDWATER AND RELATED STATISTICAL APPROACHES

Depending on the available information at hand, a number of statistical techniques can be applied to interpret CECs occurrence data. They range from the relatively simple, like linear regression to more complex tools like canonical correlation analysis (*Table 4*).
It means in some cases just simple studies, as correlation of concentration data with some of the parameters described above (width of unsaturated zone, for example) can be done.
Despite the limited scope of this type of study, these associations can provide valuable information about some of the key parameters.

Occurrence of emerging contaminants in groundwater and related statistical approaches										
	Cor	CA	CCA	CT	RST	Kr	MLR	PCA	PMF	VP
Co-occurrence	●									
Detection frequency				●						
Difference in concentration					●					
Source-tracking	●							●	●	●
Interrelation of factors			●							
Spatio-temporal relationship		●				●	●	●		
Prediction of GW concentration	●					●	●			

Table 4: Summary of CECs groundwater occurrence and related statistical approaches

Cor=Correlation, CA=Cluster analysis, CCA= Canonical correlation analysis, CT=Contingency tables, RST=Rank Sum Test, Kr=Kriging, MLR=Multiple regression, PCA=Principal Component Analysis, PMF=Positive Matrix Factorization, VP=Variation Partitioning

To date, few comprehensive regional studies have analysed factors affecting CECs distribution in groundwater. Menció and Mas-Pla (2019) studied fate of antibiotics in groundwater; finding that total amount of explained variation is very low. The authors highlight the need to include sorption and degradation as key parameters, among others.

In a study carried out in three Municipal Solid Waste landfills and three Wastewater Treatment Plants located at northeast Poland to determine occurrence of CECs in water, Kapelewska et al. (2018) found that CECs in groundwater primarily emanated from infiltration of landfill leachate, while sewage treatment plants were the principal origin of CECs in surface water.

5.1 Co-occurrence of contaminants

One of the most powerful tools to draw conclusions consists in analysing the relationship between at least two variables by means of correlations.
This technique of information analysis provides the strength and sense of the relationship. In the survey of Iowa Groundwater (IDGR, 2015) tritium (indicating recent recharge) has been used as a predictor of the occurrence of pesticide and acetanilide degradates. Otherwise, Hepburn et al. (2019) provide indications that PFOA/∑PFAA is a useful tracer of municipal landfill derived PFAS when strong correlation with ammonia exists.
Cluster analysis have been used to identify groups in which observations are more similar. Elliot et al. (2017) used cluster analyses to reveal chemicals that frequently co-occurred such as pharmaceuticals and flame retardants at sites receiving similar inputs such as wastewater treatment plant effluent.

5.2 Detection frequency

Some CECs detected in groundwater have turned out to be relatively ubiquitous, being present in water, soil and sediments, while different ones show a low detection frequency. Frequency of detection in each region, together with the quality and quantity of available data has been suggested (Montagner et al., 2019) for the elaboration of priority lists in order to choose few indicators from the large amount of non-regulated contaminants. Elliot et al. (2017) selected the 30% threshold of detection frequency to reduce the dataset to CECs that are fairly ubiquitous across the Laurent Great Lakes Basin. In the study of Bexfield et al. (2019), contingency tables were used to test for differences in detection frequencies among compounds or sites.

5.3 Difference in concentration

In the study of Bexfield et al. (2019), rank sum tests were performed to test for differences in the distribution values for compounds or sites in a systematic assessment of hormones and pharmaceuticals in groundwater across the United States. Among the most significant results, it is worth noting that wells with a detection were significantly shallower and had significantly higher ^{3}H concentrations than wells without a detection.

5.4 Source-tracking

Identification of CECs potential source contributions is essential for modelling fate and transport of emerging contaminants, so a number of studies have been carried out to reduce high uncertainties associated to their sources and inputs. Garcia-Gil et al. (2018) have studied correlation between NO_3 and occurrence of antibiotics, in an attempt to provide evidence that antibiotics originate from the sewage network. In the same work confirmation of higher pH in groundwater samples containing UV-filters was reported. In some instances, groundwater concentration of emerging contaminants is due to recharge from polluted rivers, which emphasizes the need to build a solid conceptual model. Lamastra et al. (2016) propose carbamazepine, galaxolide and sulfamethozale, between the CECs, as environmental tracers to identify sources and pathways of contamination/pollution. Yu's (2019) study shows the suitability of artificial sweeteners as indicators of raw wastewater contamination in urban surface water/groundwater.

Variation partitioning was introduced by Borcard (1992) to analyse correspondence between a response variable (occurrence of emerging contaminants in groundwater) and several data sets of environmental properties (physical, chemical, climatic, etc.). The methodology consists of apportioning the variation of the response variable among the different data sets.

Principal component analysis has been used to identify sources of emerging contaminants (Karpuzcu et al., 2014). It provides a new set of uncorrelated variables by transforming the original variables that overcomes problems associated to correlation among chemicals.

In the cited study, one component is indicative of urban/residential use, associated to cotinine, DEET, carbamazepine, erythromycin and sulfamethoxazole, while other explained presence of atrazine, metolachlor and acetochlor (agricultural). The principal components are ordered. Depending on the amount of variance explained by main components, the sources of emerging contaminants can be categorized.

Receptor modelling combines Principal Component Analysis with Multiple Linear Regression (PCA-MLR) to obtain a regression model in terms of those variables, which contribute the most to PCA (Jiang et al., 2015).

Positive Matrix Factorization is a multivariate factor analysis method targeted to identify factors representing major emission sources. Scores on these factors are then regressed against the concentrations to estimate the contributions from each source. In Guo et al. (2017), dominant groundwater pollution sources, differentiating between anthropogenic activities of agricultural and industrial pollution and natural factors are identified.

5.5 Interrelation of factors

In order to analyse the link between different factors, like soil properties and water well characteristics, for instance, canonical correlation analysis has been used in a number of studies. Zhang et al. (2013) performed this technique among surface water, municipal wastewater and swine wastewater.

5.6 Spatio-temporal relationships

Spatial prediction of groundwater quality in aquifers implies interpolation of available measurements. Estimation of concentration in non-sampled points is a key point to get an overall picture of the spatial distribution and develop uncertainty maps.

Geostatistical methods have been used to predict values by using several interpolation methods. The estimate of the probability of exceeding a reference limit (Luque-Espinar et al., 2018), e.g. limit of detection, limit of quantification, drinking water standard, maximum contaminant level or any other health-based screening level can be done by means of indicator kriging (*Figure 5*) in an optimal way.

Likewise, other cut-off limits can be established according to the objectives of the investigation. While spatial distribution of emerging contaminants (like consumer and personal care products) has been studied in a variety of cases in soil (Froger et al., 2021), sediments, sludge, surface water and the unsaturated zone (Corada-Fernández et al., 2015), specific studies focused on groundwater are needed in order to assess the influence of other factors and their spatial distribution.

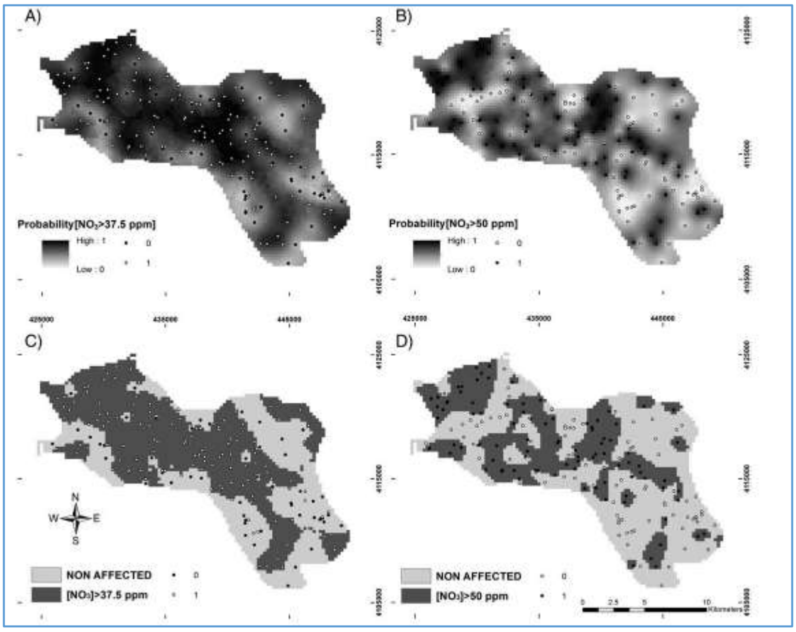

Figure 5: Probability of exceeding environmental thresholds by means of indicator kriging

A key component of any exposure study (Luque_Espinar et al., 2018) is a reliable model of the spatial distribution of the studied elements. Kriging has been used in McGuire (2013) to create maps of the spatial distribution of PFASs at an abandoned fire protection training area.

5.7 Prediction of groundwater concentration

Regression modelling may be used to study one set of factors. For instance, the occurrence of contaminants in groundwater could vary as a function of soil properties. In most cases, there are correlations among factors, so a proper analysis must be accomplished to model the relationship.

In one of the few surveys conducted in groundwater, Menció and Mas-Pla (2019) analyse the occurrence and fate of antibiotics in an alluvial aquifer of Catalonia. In the study, antibiotic occurrence in groundwater is the response variable, while antibiotic sources (human and veterinary), aquifer susceptibility (soil type and geological unit) and groundwater properties are the three explanatory variables that were used.

Multivariate regression models have been used in the work of Ayotte et al. (2012) to estimate probability of arsenic occurrence in groundwater using geologic, geochemical, hydrologic and anthropogenic data as predictor variables by means of multivariate logistic regression models.

6 REPORTING LIMITS

Emerging contaminants can be found in groundwater in a wide range of concentrations (Karpińska and Kotowska, 2021; Montesdeoca-Esponda et al., 2021). Quantification of substances in such low concentrations can pose significant analytical challenges.
In response to this need new analytical methods have been developed, aiming to measure the occurrence and concentration of water pollutants. In this situation, the information available on the concentration of certain substances is that their value is somewhat between zero and the detection or reporting limit.
Reporting limit represent the smallest concentration of a chemical that can be reported by a laboratory below which data are documented as non-detects. Several terms are used to describe different levels: critical value, limit of detection (LOD) and quantitation limit (LOQ). The first two are frequently utilised as synonyms, while the latter refers to the situation when laboratories can quantify the environmental samples concentrations with a degree of certainty (the detection limit times a safety factor selected by the laboratory to account for the occasional variation in laboratory instrument sensitivity. Often it is a value much higher than the detection limit).
Different laboratories employ different methods to determine reporting limits, and organisms in charge of the evaluation of environmental sampling have adopted various guidelines.

In conclusion, caution must be taken when comparing concentration in groundwater from different laboratories

6.1 Method detection limit (MDL)

EPA uses the term MDL, defined (USEPA, 2016) as the minimum concentration of a substance that can be measured and reported with 99% confidence that the analyte concentration is greater than zero, and is determined from analysis of a sample in a given matrix containing the analyte. In practical terms, MDL is about three times the standard deviation of results around the analyte true concentration. This value is called critical value (*Figure 6*), and protects again false-positive rate. The MDL procedure is not applicable to measurements where low-level spiked samples cannot be prepared.
A minimum of seven spiked samples and seven method blank samples is required, and MDL of both sets are calculated as follows:

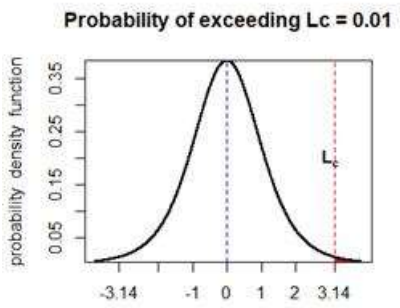

Figure 6: Critical value

$MDL_s = t_{(n-1,1-\alpha=0.99)}S_s$ *Equation 1*

$MDL_b = \acute{\chi} + t_{(n-1,1-\alpha=0.99)}S_b$ *Equation 2**

*Equation 2 is applicable if all blanks have numerical results. If not, highest blank result or 99th percentile is used instead

Where:

MDL_b = the MDL based on method blanks

MDL_s = the MDL based on spiked samples

$\acute{\chi}$ = mean of the method (blank or spiked) results

$t_{(n-1,1-\alpha=0.99)}$ = Student´s t-value

S_b,S_s = Standard deviation of blank or spiked samples

The greater of MDL_b or MDL_s is selected as the initial MDL. Further details are provided in USEPA (2016).

6.2 Quantification limit (QL)

The Quantification limit is calculated as ten times the standard deviation used in the method detection limit (USEPA, 2016), although other organizations (Helsel, 2012) use twice the detection limit. The resulting threshold is approximately three times the value of the USEPA detection limit.

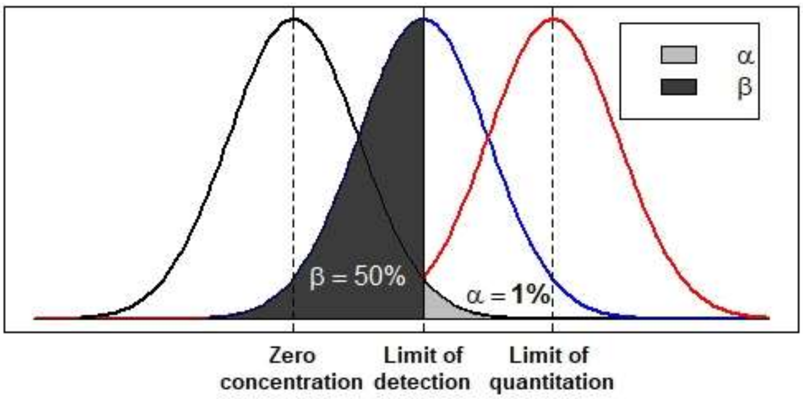

Figure 7: *Relationship between Limit of Detection and Limit of Quantitation (Helsel, 2012)*

Since the measurement uncertainty plays an important role in decision-making, the quantification (or quantitation) limit is frequently used in statistical testing. Below the quantitation limit uncertainty increases rapidly, becoming about 50% at the limit of detection (*Figure 7*).

6.3 Multiple comparison problem (interlab comparison)

In order to assess the reliability of tests results and determine their uncertainty, interlaboratory comparisons (ILCs) are commonly performed. Because CECs are numerous, the problem of multiple comparisons arises, involving a large number of statistical tests. In this situation, significant results (differences between two laboratories) might happen by chance. This kind of error is called a Type 1 error, also known as a “false positive”.

While the classic approach to counteract this problem, the Bonferroni correction, (Miller, 1981) attempts to set the familywise error rate (probability of getting at least one false significant result) to 5%, there are alternative approaches based on maintaining the rate of false positives without inflating the rate of false negatives.

McGuire (2013) proposes Benjamini-Hochberg adjustment (Benjamini and Hochberg, 1995) for multiple testing to control Type 1 error rate in inter-lab comparison. To test for significant differences between the concentrations measured at each laboratory, a series of matched pair t-tests were conducted on log-transformed concentration data from the selected laboratories.

6.4 Censored values

Under article 17 of the Water Framework Directive, the European Union was required to establish a framework to prevent and control groundwater pollution, including the derivation of Environmental Quality Standards (EQS) and threshold values. When there is a mixture of censored and non-censored data, as it is usual with CECs concentration data, the problem of how to calculate descriptive statistics (mean, median and standard deviation) arises (see Lapworth et al., 2019 re treatment of censored data).

Before processing values for analysis, data manipulation operations are required. First of all we need to store censored values in a database, and then perform data filtering and cleansing tasks, like removing any duplicate values.

Raw data may come in different units (mg/L, ng/L, µg/L), so it is necessary to ensure that values are properly formatted and homogenized.

A key point for data processing is the encoding of values, so that it is possible to know if a value is below the reporting limit. Several procedures have been described (Helsel, 2012), like indicator variables or interval endpoints.

Taking into consideration the distinctive characteristics of censored groundwater concentration data, appropriate statistical tests are required. In the comprehensive study of Helsel (2012), a comparison between substitution, maximum likelihood and other specific methods, like robust regression on order statistics or survival analysis (Kaplan-Meier method) is completed.

In this regard, Annex IV of the Groundwater Directive (Council Directive 2006/118/EC) sets that all measurements below the quantification limit have to be substituted by half of the value of the highest quantification limit, except for total pesticides.

Although in some cases, it is possible to estimate mean values in censored data sets with a single reporting limit, its replacement distorts estimates of the standard deviation (Helsel, 2012), and therefore confidence limits used to check compliance with threshold values.
Analogously to the procedure used to verify compliance with standards in the absence of censored values, the elaboration of confidence intervals is the reference method to verify compliance with standards or thresholds when some values are below the reporting limit.
In case the objective of the study is to demonstrate the presence of some CEC, the procedure is to compare the mean concentration with the quantification limit.
When all values are below the reporting limit, the confidence level of the proportion of measurements below the reporting limit can be estimated based on binomial probabilities (Helsel, 2012).
For example, for a dataset of 10 measurements, the confidence interval for the true proportion of censored observations lies between 0.74 and 1, what means that less than 26% of observations are expected to exceed the reporting limit. If the size of the dataset is just five, the confidence interval is (0.55, 1). In this case, less than 45% of observations are expected to exceed the reporting limit.

7 BACKGROUND QUALITY AND COMPLIANCE TO STANDARDS

Background values are a key element in the process of characterization of groundwater bodies, especially to derive threshold values.

According to the Groundwater Directive (Council Directive 2006/118/EC, Article 2.5), background level means the concentration of a substance or the value of an indicator in a groundwater body in the absence of altered anthropogenic conditions in relation to natural conditions. In the strict sense, it refers to conditions relating to pre-industrial times, which does not realistically represent actual conditions. Emerging contaminants may span from natural to man-made or manufactured substances whose presence has been suspected or proved in various environmental compartments. For non-naturally occurring substances, such as synthetic emerging contaminants, the background level must be set to zero. Various methodologies are available to determine if representative concentration of CECs in groundwater is greater than the MQL. The signal-to-noise approach has been used (Kibuye et al., 2019) to determine the MQL, using ten times over background as a basis for its calculation.

The most accepted is the development of confidence intervals. The procedure consists in estimating the mean (or median) of the population by means of the sample, calculating an interval in which its true value is expected to be included instead of estimating the parameter using a unique value.

There are a number of conditions to be met by any dataset in order to calculate a confidence interval, among which include statistical independence, stationarity, lack of outliers and adjustment to the distributions (required in case of parametric tests). Independence implies the nonexistence of autocorrelation or trends in data, which generally requires a low sampling rate and a minimum number of samples between 8 and 10 (USEPA 2009).

As pointed out in previous paragraphs, concentration of synthetic CECs must equal zero, which implies the elaboration of a confidence limit. Then upper confidence limit must be less than the method quantification limit (MQL).

8 SUMMARY OF TECHNIQUES

Table 5 provides a summary of statistical methods that can be used to interpret CECs data and metadata in groundwater.

(Statistical) *Method*	*Technique*	*Premises*	*Process or aim*
I. Canonical correlation	a. Canonical correlation analysis	Interpretation of canonical variate scores not easy	Links between different factors
II. Censored methods	b. Robust regression	Just one reporting limit	Elaboration of confidence intervals of percentiles, check compliance to standards, probability of exceedance the reporting limit
	c. Kaplan-Meier	Several reporting limits	
III. Cluster analysis	d. Hierarchical clustering	Rank transformed data	Co-occurrence of contaminants, sites with similar CECs signatures
IV. Correlation tests	e. Pearson correlation test	Bivariate normal density	Associations between two variables (conc.-gw quality, seasonal variation, variations in distribution, etc.)
	f. Spearman correlation test	Monotonic relationship	Associations between two variables (conc.-gw quality, seasonal variation, variations in distribution, etc.)
V. Difference between groups	g. t-test	Normality, two groups	Difference between two groups
	h. Wilcoxon rank sum test	Two groups	Influence of land use on concentration, differences in the distribution values
	i. Analysis of variance	Normality, more than two groups	Seasonal variation
	j. Kruskal-Wallis	More than two groups	Seasonal variation
VI. Geostatistics	k. Ordinary kriging	Layers projected in same coordinate system	Interpolation of values, development of uncertainty maps
	l. Indicator kriging		Spatio-temporal relationships, probability of exceeding a reference limit
VII. Graphical analysis	m. Superposition of GIS layers	Layers projected in same coordinate system	Depth of unsaturated zone Aquifer type Type of monitoring station Land use
VIII. Multivariate factor analysis	n. Positive Matrix Factorisation	Slower computing time. More complicated than PCA	Estimate contribution from different sources
IX. Multiway tables	o. Contingency tables	More than two categorical variables difficult to analyse	Interactions between variables, differences in detection frequencies
X. Regression modelling	p. Multiple linear regression	Multi-Collinearity of variables can cause problems	Several explanatory variables, like sources, soil type and groundwater properties to account for occurrence
	q. Receptor modelling	Combines PCA and Multiple Linear Regression	Identification of variables that contribute to PCA
XI. Variation partitioning	r. PCA + VP	PCA scores used as VP parameters	Variation of concentrations as a function of explanatory variables

Table 5: Methods to calculate CECs data and metadata

9 CONCLUSIONS AND MONITORING RECOMMENDATIONS

A large number of different kinds of chemicals are increasingly being detected in the European aquatic environment. The relatively high cost of taking groundwater samples is one of the main reasons why many of them are not commonly monitored. Accordingly, their groundwater occurrence and distribution across Europe is poorly characterised and available data on their occurrence, fate and transport is limited.

Methods for sampling and analysis are dedicated to a limited number of known CECs. Even for these, data are still scarce and highly scattered. That is the reason why, in certain cases, spatial correlation has been found for common contaminants, like nitrates, but not for other abundant substances, like pesticides or antibiotics.

Hence, it seems essential to prioritise monitoring locations in order to minimise uncertainties caused by limited sampling. The Watch List under the Environmental Quality Standards Directive (Council Directive 2008/105/EC) includes a number of potential water pollutants for which the available information is either insufficient or of insufficient quality for an EU-wide risk assessment.

Despite the positive efforts that have been made to develop the Groundwater Watch List, a policy development is strongly required, to tackle the study of the numerous substances present in groundwater and understand in this way its temporal and spatial variation.

Taking into consideration the rapid development of the state of the art and the limited resources available, a prioritisation scheme is needed. The use of indicators, attempting to identify the most important compounds or class of compounds, or specific pollution processes, is a feasible alternative to address target and non-target screening.

As a means of achieving effectiveness of groundwater monitoring programmes, comprehensive knowledge of physical processes jointly with the purpose and objectives of monitoring are required.

The first and most critical step to improve their efficiency, before reaching any conclusion, is the elaboration of a sound hydrogeological conceptual model. It is required as a prior condition to any interpretation of data. Moreover, it is essential to represent both the groundwater flow system, including surface water/groundwater interactions, and the physical system. For that we need to consider primary factors, additional drivers, features of prevalent contaminant and source area processes.

Among the primary factors, Soil properties (Organic carbon content, pH and clay content), the properties of the Physical Structure (Lithology), Aquifer and Groundwater properties (Groundwater parameters, Unsaturated zone thickness, Hydraulic conductivity, Age, pH, Redox conditions, DO), Hydrological processes (Relationship river-aquifer, Climate, Flow condition and Seasonal variation) have proved to be useful for the posterior interpretation of data, so they must be considered and recorded whenever possible.

Referring to additional drivers, Land use, the spatial character of the focus of pollution and Groundwater well characteristics are the key factors. For example, over-pumping of large volumes of water is likely to induce the release of pore water with high CECs concentration.

In conjunction with the previous factors, Physico-chemical properties of the contaminants (Water solubility, Acid dissociation constant, Structure and size and Hydrophobic interaction) and Interaction with other contaminants (Synergistic effects, NAPL-water partitioning and NAPL-water interfacial adsorption) are also influential factors.

Depending on the objective of the study and the amount of information available, different statistical techniques can be used to analyse distribution and concentration of emerging contaminants in groundwater, ranging from simple visualization techniques to sophisticated methods or combination of them.
Exploratory analysis is the first stage in such analysis and a valuable tool to explore the sample data and summarize their major features. Some processing is then required, like transformation to reduce skewness of data or fitting a variogram model to identify spatial autocorrelation or global trends.
Guidelines for the establishment of quality standards (threshold values or maximum contaminant levels), taking into account local environmental settings are required for key contaminants; otherwise monitoring programmes will simply ignore their existence.
Frequency of detection of emerging contaminants is highly variable, depending on their concentration and the method detection limit. Considering the range of concentrations observed in groundwater, with an upper bound being of the order of ng/L, it is necessary to apply appropriate statistical techniques to obtain summary statistics of censored values.
The quantification (or quantitation) limit is frequently used in statistical testing, so detection or quantitation limit must be provided jointly with lab concentration data to avoid bias in results.

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