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Analysis of complex regional databases and their support in the identification of background/baseline compositional facies in groundwater investigation: developments and application examples

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ABSTRACT

The management of groundwater resources has become a matter of public interest during recent years. It is a difficult and sensitive topic for all involved subjects, scientists, state agencies, public and private water supply companies and citizens. Therefore, tools for collection, storage, evaluation and public visualization of groundwater-relevant information have to be constructed and implemented. The development of network-based technologies, and the support of the Geographical Information Systems, would help the dissemination of the knowledge about groundwater chemistry, as well as the integration of the geochemical data with other type of information (geological, hydrogeological, soil use, etc.). However, dedicated repositories often contain fragmented numerical and categorical information from different sources obtained for dissimilar aims and divergent interests, thus compromising a holistic management of the resource. Given the complicated nature of the information related to groundwater and geochemical behavior, statistical methods describing and evaluating data patterns in complex regional databases have to be developed in a dedicated way. An application example is presented for the Geobasi–Tuscany (central Italy) project, a repository where all the information about the geochemistry of natural media, including groundwater, collected in the regional territory is stored. Robust methods, not sensible to anomalous cases, have been associated to the compositional approach, leading to the identification of the baseline compositional facies, related to frequent and spatially diffused geochemical phenomena. The facies have been discriminated from the other ones, related to specific environmental conditions, affecting limited portions of the territory. The methodology can be easily integrated with those based on the classical ternary or square diagrams for the identification of the hydrochemical facies. The proposed robust approach, compositional and, therefore, multivariate, appears to be an efficient way to understand how the natural and not natural processes are working on a regional scale.

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1. Introduction

Groundwater, the most important fresh water resource, is susceptible to contamination due to natural and anthropogenic sources. Since most of the world's population depends on groundwater sources for drinking water supply and other uses (Oki and Kanae, 2006), degradation of its quality due to contamination is of serious concern in both developed and underdeveloped countries. The prevention of groundwater contamination is generally the preferred action, rather than the removal of the pollutant once it has entered the aquatic environment. Hence, it is crucial to delineate areas that are vulnerable to groundwater contamination and thus take suitable precautionary measures. In this framework, it is important to collect large quantities of groundwater data and to organize them in dedicated repositories including information collected about different substances on variable spatial and temporal scales. However, when the work is performed at regional scale, and the sources of information are related to different data input (e.g., public agencies, academic institutions, private companies), a fragmented view of groundwater conditions is obtained. Each source in fact contributes to a restricted domain of a more general problem since planned for different aims (Khalil et al., 2014). Fragmented non-harmonized databases are thus difficult to integrate and often provide incomplete information to decision-makers (Chesnaux et al., 2011; Lavoie et al., 2015; Pascal-Gonzales et al., 2015; Singh, 2014). In this paper, a methodology to explore the geochemical information contained in a multi-source complex repository, developed jointly

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with Tuscany Region (central Italy) administration, is proposed (Raco et al., 2015). The approach is based on the use of compositional data analysis theory (Aitchison, 1986) implemented by the adoption of robust tools (Verboven and Hubert, 2005; Filzmoser and Hron, 2008) as a first attempt to identify background/baseline compositional facies associated to common geochemical processes spatially diffused or related to a well defined geological framework. These compositional facies have to be discriminated from the anomalous ones, often related to peculiar conditions affecting limited portions of the territory and related to restricted geochemical conditions.

In this perspective, the approach does not consider single variables one by one, but the joint behavior of the whole water composition as expressed by its major anions and cations. This is the sense of the proposed concept of 'compositional facies' with respect to the traditional one (Al-Bassam and Khalil, 2012; Durov, 1948; Giménez-Forcada et al., 1999; Piper, 1944, Giménez-Forcada, 2014).

The method is able to combine geological and hydrogeological information with geochemical indices to obtain maps of groundwater hydrochemical conditions. The resulting maps allow the understanding, at a first attempt and on a regional scale, of the dynamics of the processes affecting groundwater resources and their spatial behavior.

1.1. Groundwater protection: the conceptual model

Groundwater protection is a priority for human health as established by the environmental organizations and institutions of many industrialized and developing countries (UN-Water, 2011; WHO, 1992). The safety and accessibility of drinking water are in fact major concerns throughout the world. Health risks may arise from consumption of water contaminated by infectious agents, toxic chemicals and radiological hazards. Groundwater contained in aquifers is one of the most important sources of water on Earth: recent estimates by international and European institutions report that about 30% of our freshwater is groundwater. The rest is found on the surface in streams, lakes, rivers and wetlands. Most of the world's freshwater — about 69% — is locked away in glaciers and ice caps. Forecasts of FAO (Food and Agriculture Organisation of the United Nations) and WHO report that 1.8 billion people will experience absolute water scarcity in 2025, placing 2/3 of the world under water-stressed conditions and that by 2030 almost half the world will live under conditions, of high water stress (GLAAS Report, 2014).

The European Community's Water Framework Directive (WFD) 2006/118/EC (EC, 2006) was drafted with the aim to prevent and control European groundwater pollution. It includes procedures to define: i) criteria for assessing the chemical status of groundwater; ii) criteria for identifying significant increasing trends in groundwater pollution levels, and iii) actions for preventing and limiting discharges of pollutants into groundwater. The main goals of WFD are to achieve an acceptable chemical and quantitative status of groundwater by 2016. This target can be considered realistic when a description, inclusive of all the features able to provide a 'conceptual model' at the aquifer scale and the relationships with the surrounding systems (boundary conditions), are properly described and taken into account. With this approach, useful integrated tools can be provided to support local public authorities for viable decision-making processes. As a consequence, (i) geological aspects, (ii) nature of the recharging areas, (iii) features of the main water flow circuits, (iv) hydrogeological and hydrogeochemical characteristics, and (v) water vulnerability conditions are all descriptors of these complex geochemical systems. In this context, the presence of a repository, where the chemical information is stored and can be linked with other types of data, is the starting point from which any other analysis can be developed and implemented, such as the determination of background/baseline values, a fundamental tool to understand how natural processes work, and to identify the effect of anthropogenic factors in time and space. Their knowledge is often useful to orient political decisions concerning the governance of environmental problems (e.g., quality of potable water, reclamation of polluted sites). However, the concept of background/baseline is univariate, and aims to give reference values for each chemical component independent from the other terms of the chemical composition.

1.2. The "compositional" concept of background/baseline hydrochemical facies

The aim of this research is to propose a methodology to identify the background/baseline geochemical facies for groundwater chemistry in a compositional sense (Aitchison, 1982; Buccianti, 2013) and, therefore, multivariate. The approach is alternative to the use of trilinear diagrams, as proposed by Piper (1944) and to a lesser extent by Durov (1948), to recognize hydrochemical facies. It is also alternative to the univariate partitioning of geochemical frequency distributions to recognize subsets of data (Sinclair, 1974, 1989, 1991). A composition is, in fact, given by D variables, determined on the same sample where the measured unit is typically able to give only the proportion of each component of the same whole (e.g., %, ppm, mg/L). The target was achieved working on data stored in the GEOBASI repository, a very large database (6808 groundwater and spring samples characterized by the major ions) compiled to include all the numerical and categorical information under the umbrella of the GEOBASI-Tuscany project, managed by the Tuscany Region (Central Italy) administration (Raco et al., 2015). Data stored in the database are derived from several reports and scientific publications of public and private institutions, produced for different projects and aims, and cover a wide span of time, from 1977 to 2009. The spatial distribution of the samples cannot be considered homogeneous, a condition that hinders the use of standard geostatistical methods on a wide regional scale. Other significant drawbacks of the database are that (a) the groundwater samples were not collected and analyzed by harmonized methods, and (b) there is no quality control information, which are necessary prerequisites for the development of a harmonized hydrogeochemical database (Reimann and Birke, 2010).

The investigation of the structure of the chemical information contained in the GEOBASI-Tuscany database was performed by using methods coherent with the sample space of compositional data (Aitchison, 1986; Buccianti, 2013; Buccianti and Magli, 2011). Thus, taking into account the proportionality underlying concentration values in the appropriate geometry for statistical analysis. Moreover, due to the expected presence of anomalous values and inherent high heterogeneities in the database, robust methods to estimate central tendency parameters and variance–covariance structure were adopted (Daszykowski et al., 2007; Maronna and Zamar, 2002; Rousseeuw, 1984; Verboven and Hubert, 2005).

The approach is devoted to discovering which areas of the regional territory geochemical processes compatible with the nature of the rocks are expected to govern the chemistry of groundwater, their frequency and spatial diffusion (Buccianti and Gallo, 2013; De Caritat and Grunsky, 2013). The identification of these processes, and the discrimination from rare or spatially limited (punctual) phenomena, represents the first step to evaluate the possibility to define background/baseline geochemical facies in a compositional sense.

The diagnostic chemical character of water solutions in hydrologic systems is often determined by the application of the concept of hydrochemical facies. It represents a convenient subdivision of water compositions by identifiable categories, and reflects the effect of chemical processes occurring between the minerals within the subsurface rock units and the groundwater (Chaudhuri and Ale, 2013; Nwankwoala et al., 2011). However, this approach although neither compositional nor multivariate, was used here to describe the geochemical features of the investigated waters from the common perspective. Starting from this point our aim is to move towards the concept of background/baseline geochemical facies in a compositional and, therefore, multivariate framework (Guler and Thyne, 2004).

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