# GIS-based hydrogeological platform for sedimentary media

PhD Thesis

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### I. ABSTRACT

The detailed 3D hydrogeological modelling of sedimentary media (e.g. alluvial, deltaic, etc) that form important aquifers is very complex because of: (1) the natural intrinsic heterogeneity of the geological media, (2) the need for integrating reliable 3D geological models that represent this heterogeneity in the hydrogeological modelling process and (3) the scarcity of comprenhensive tools for the systematic management of spatial and temporal dependent data.

The first aim of this thesis was the development of a software platform to facilitate the creation of 3D hydrogeological models in sedimentary media. It is composed of a hydrogeological geospatial database and several sets of instruments working within a GIS environment. They were designed to manage, visualise, analyse, interpret and pre and post-process the data stored in the spatial database

The geospatial database (HYDOR) is based on the Personal Geodatabase structure of ArcGIS(ESRI) and enables the user to integrate into a logical and consistent structure the wide range of spatio-temporal dependent groundwater information (e.g. geological, hydrogeological, geographical, etc data) from different sources(other database, field tests, etc) and different formats(e.g. digital data, maps etc). A set of applications in the database were established to facilitate and ensure the correct data entry in accordance with existing international standards.

The set of analysis tools was developed as an extension of ArcMap environment (ArcGIS; ESRI). This set of tools was separated into three main modules represented by different toolbars.

The first toolbar, termed HEROS, allows the user to exploit the geological data stored in the database and facilitate the generation of 3D geological models. Detailed stratigraphic columns of the selected boreholes can be generated using customized queries. The automatic creation of a geological profile is possible by displaying the borehole lithological columns, the geophysical and geotechnical field-test results, and the defined stratigraphic units. The user is able to analyse and to define the possible existing correlation surfaces, units, and faults on the basis of an interactive analysis environment. These spatial elements can then be converted within a 3D environment. Finally, the use of the resulting geological model to support the hydraulic parameterisation for hydrogeological modelling is also possible by employing another command.

The second toolbar, which is known as QUIMET, is composed of a set of instruments for analysis that cover a wide range of methodologies for querying, interpreting and comparing groundwater quality parameters. They include, among others, chemical time-series analysis,

ionic balance calculations, correlation of chemical parameters, and calculation of various common hydrogeochemical diagrams (e.g. Schöeller-Berkaloff, Piper, and Stiff). Moreover, it is also possible to perform a complete statistical analysis of the data including descriptive statistical univariate and bivariate analyses, the generation of correlation matrices of several components, calculation of correlation graphics, etc.

The last toolbar (HYYH) was designed to analyse and visualise different hydrogeological measurements and hydraulic field test results. Contour maps and further spatial operations of the depth or thickness of the aquifers could be generated using customized queries. Likewise, piezometric maps can be created for the selected points and for the selected period of time with another command included in this toolbar. Additionally, multi-criteria query forms enable the user to analyse and visualise different data and interpretations derived from pumping and tracer tests.

The interpreted data and calculations can be easily stored and consulted in the same platform and can be used to build an updatable model database for further interpretations. Thus, each new study does not have to start from scratch.

The second aim of this thesis is to implement this modelling platform in the urban area of Barcelona (NE, Spain) to structure all the available data and to set up a working framework of groundwater resources in terms of both quantity and quality. Concretely, in the Besòs Delta area (NE of Barcelona), the integration of the available data into the HYDOR database and the use of the aforementioned instruments and methods allowed us to: 1) delimit the geological units by means of sequence stratigraphic subdivision, 2) generate the 3D facies belt-based model of the Besòs Delta built on the basis of this geological characterisation and 3) use this model to constrain the distribution of hydraulic parameters and thus obtain a consistent hydrogeological model of the delta , which was calibrated by water management and production data recorded over the last hundreds years. Because of this marked improvement in the characterisation of the geology of the Besòs Delta complex, the lower aquifer was incorporated into the model, which significantly contributes to our understanding of the hydrogeological characteristics of the delta.

### II. RESUMEN

La modelización hidrogeológica tridimensional de los medios sedimentarios (p.ej. sedimentos aluviales, deltas) que suelen constituir acuíferos importantes es compleja debido principalmente a tres factores: (1) la heterogeneidad natural intrínseca del medio, (2) la necesidad de integrar un modelo geológico tridimensional que represente dicha heterogeneidad adecuadamente en los procesos de modelización hidrogeológica y (3) la escasez de herramientas apropiadas para gestionar grandes cantidades de datos hidrogeológicos espacio- temporales.

El primer objetivo de esta tesis ha sido el desarrollo de una plataforma software en un entorno GIS que facilite la realización de modelos hidrogeológicos 3D. Está compuesta por una base de datos geoespacial y un conjunto de herramientas que permiten al usuario gestionar, visualizar, analizar, interpretar y pre-post procesar los datos almacenados en dicha base de datos.

El modelo de bases de datos propuesta en esta tesis (HYDOR) se ha implementado en una base de datos geoespacial del tipo *Personal Geodatabase* (ArcGIS, ESRI) y permite la integración en una estructura coherente y lógica de un amplio rango de tipos de información hidrogeológica procedentes de diversas fuentes y con diferentes formatos.

Los diferentes instrumentos desarrollados para explotar los datos almacenados en la base de datos se han creado como una extensión de ArcMap (ArcGIS; ESRI) y se reagrupan formando tres barras de herramientas.

La primera barra de herramientas (HEROS) además de facilitarnos el análisis y la interpretación de los datos geológicos almacenados en la base de datos, nos permite generar modelos geológicos tridimensionales. Entre las funciones de dichas herramientas, está la de poder visualizar la información geológica aportada por los sondeos en forma de columna estratigráfica así como la generación automática de perfiles geológicos que muestran las diferentes columnas estratigráficas de los sondeos seleccionados. Información útil como los resultados de los ensayos geofísicos así como las unidades geológicas definidas aparecen también en la pantalla del mismo perfil geológico. Este entorno es óptimo para que el usuario analice y defina las superficies de correlación, las diferentes unidades geológicas y las posibles fallas. Estos elementos espaciales se pueden visualizar en tres dimensiones. Finalmente, otra herramienta nos proporciona la parametrización hidráulica inicial (para el modelo hidrogeológico) de las diferentes unidades geológicas partiendo de las características texturales de las mismas.

La segunda barra de herramientas, QUIMET, cubre un amplio rango de metodologías para consultar, interpretar y comparar diferentes parámetros hidroquímicos. Además nos

permite desarrollar un análisis estadístico completo en el que se incluyen entre otros, análisis estadísticos univariante, bivariante y generación de matrices de correlación de diferentes compuestos químicos.

La última barra de herramientas (HYYH) se ha diseñado para visualizar y analizar los datos hidrogeológicos entre los que se incluyen los procedentes de ensayos hidráulicos. Usando estas herramientas se pueden generar mapas de isolineas y otras representaciones espaciales que nos permitan visualizar la profundidad o el espesor de los acuíferos. Del mismo modo, se pueden obtener mapas piezometricos de los puntos seleccionados para un intervalo de tiempo determinado por el usuario. Finalmente, otra herramienta nos permite consultar las interpretaciones procedentes de ensayos hidráulicos.

La información obtenida usando todas estas herramientas, también se almacenan en la base de datos constituyendo de este modo una base para futuras interpretaciones.

El segundo objetivo de esta tesis ha sido la aplicación de esta plataforma software en la gestión de los datos disponibles del área urbana de Barcelona (NE de España) obteniendo con ello una herramienta apropiada de gestión de los recursos hídricos de esta zona tanto en términos de calidad como de cantidad.

Concretamente en la zona del Delta del Besòs (NE de Barcelona), la aplicación de esta plataforma de gestión nos ha facilitado lo siguiente: (1) la delimitación de unidades geológicas basadas en criterios de estratigrafía secuencial, (2) la generación de un modelo geológico tridimensional de facies basado en dichos criterios estratigráficos, (3) el uso del modelo geológico obtenido par establecer la distribución espacial de los parámetros hidráulicos que nos han servido para generar un modelo hidrogeológico consistenete del complejo deltaico. Este modelo se ha calibrado además con datos incluidos también en la base de datos y que proceden de diversos puntos tanto de gestión como de producción durante de los últimos 100 años.

Todo esto ha supuesto una mejora significativa en la caracterización geológica del Delta del Besòs lo que nos ha llevado a mejorar su caracterización hidrogeológica.

### III. RESUM

La modelització hidrogeològica tridimensional dels mitjans sedimentaris que solen constituir aqüífers importants (p.ex. sediments al·luvials, deltes) és complexa. Això es deu principalment a tres factors: (1) l'heterogeneïtat natural intrínseca del medi, (2) la necessitat d'integrar un model geològic tridimensional que representi adequadament l'heterogeneïtat en els processos de modelització hidrogeològica i (3) l'escassetat d'eines apropiades per gestionar grans quantitats de dades hidrogeològiques espai-temporals.

El primer objectiu d'aquesta tesi ha estat el desenvolupament d'una plataforma software en un entorn GIS que faciliti la realització de models hidrogeològics 3D. Està composta per una base de dades geoespacial i un conjunt d'eines que permeten que l'usuari gestioni, visualitzar, analitzi, interpreti i pre-post processi les dades emmagatzemades en la base de dades.

El model de bases de dades proposada en aquesta tesi (HYDOR) s'ha implementat en una base de dades geoespacial de tipus *Personal Geodatabase* (ArcGIS, ESRI), que permet la integració d'un ampli rang de tipus d'informació hidrogeològica procedents de diverses fonts i formats en una estructura coherent i lògica.

Les diferents eines desenvolupades per l'explotació de les dades emmagatzemades a la base de dades s'han implementat com una extensió d'ArcMap (ESRI). Aquestes eines es reagrupen en tres barres diferents.

La primera barra d'eines, HEROS, ens permet analitzar i interpretar les dades geològiques emmagatzemades a la base de dades, permetent alhora la creació de models geològics tridimensionals. També s'han desenvolupat eines que permeten visualitzar la informació geològica aportada pels sondejos en forma de columna estratigràfica, així com generar automàticament perfils geològics per mostrar diferents columnes estratigràfiques de sondejos preseleccionats. A la pantalla del mateix perfil geològic també apareix informació útil com són els resultats dels assaigs geofísics o les unitats geològiques definides. Aquest entorn és òptim perquè l'usuari analitzi i defineixi les superfícies de correlació, les diferents unitats geològiques i les possibles falles. Els elements espacials definits es poden visualitzar en tres dimensions. Finalment, una altra eina ens proporciona la parametrització hidràulica inicial de les diferents unitats geològiques (per al model hidrogeològic) partint de les seves característiques texturals.

La segona barra d' eines, QUIMET, inclou un ampli rang de metodologies de consulta, interpretació i comparació de diferents paràmetres hidroquímics. A més a més, també ens permet desenvolupar un anàlisi estadístic complet en el que s'inclouen, entre altres, anàlisis

estadístics univariant, bivariant i generació de matrius de correlació de diferents compostos químics.

L'última barra d' eines, HYYH, s'ha dissenyat per a visualitzar i analitzar les dades hidrogeològiques, entre d'altres, els procedents d'assajos hidràulics. Amb aquestes eines es poden generar mapes d'isolínies i altres representacions espacials que permeten visualitzar la profunditat o l'espessor dels aqüífers. De la mateixa manera, es poden obtenir mapes piezomètrics per a un interval de temps i de punts determinats per l'usuari. Finalment, una altra eina ens permet consultar les interpretacions procedents d'assajos hidràulics.

La informació obtinguda de totes aquestes eines s'emmagatzema a la base de dades, constituint d'aquesta manera una base per a futures interpretacions.

El segon objectiu d'aquesta tesi és l'aplicació d'aquesta plataforma software a la gestió de les dades disponibles de l'àrea urbana de Barcelona (NE de Espanya), obtenint una apropiada eina de gestió dels recursos hídrics d'aquesta zona, tant en termes de qualitat com de quantitat.

Concretament a la zona del Delta del Besòs (NE de Barcelona), l'aplicació d'aquesta plataforma de gestió ens ha facilitat (1) la delimitació d'unitats geològiques basades en criteris d'estratigrafia seqüencial, (2) la generació d'un model geològic tridimensional de fàcies basat en aquests criteris estratigràfics i (3) l'ús del model geològic obtingut per a establir la distribució espacial dels paràmetres hidràulics que ens han servit per generar un model hidrogeològic consistenet del complex deltaic. Aquest model s'ha calibrat amb dades incloses a la base de dades i que procedeixen de diversos punts, tant de gestió com de producció, durant els últims 100 anys.

Tot això ha suposat una millora significativa de la caracterització geològica del Delta del Besòs, el que ens ha portat a millorar la seva caracterització hidrogeològica.

### IV. AGRADECIMIENTOS

En primer lugar quisiera expresar mi más sincero agradecimiento a Enric Vázquez Suñè, el director de esta tesis, por sus numerosos consejos y por su paciencia tanto en el plano profesional como en el personal. Sin duda, esta tesis no hubiese sido posible sin su ayuda.

Además me gustaría agradecer a Radu Gogu la oportunidad de conocer el apasionante mundo de las bases de datos y de los Sistemas de Información Geográficas.

Por supuesto nunca podré olvidar la ayuda que el resto de los integrantes del grupo de Hidrología Subterránea de la UPC-CSIC me ha brindado durante estos últimos años. Gracias Carlos, Xavi, Jesús, Dani, Marco, Lurdes y Marteen por vuestras charlas científicas, por vuestras revisiones, por vuestros consejos y por haberme transmitido parte de vuestra sabiduría. Sobre todo me gustaría agradecer los debates, las risas, los consejos y los ánimos al resto de doctorandos (algunos ya doctores o casi doctores) que me han acompañado en esta aventura. Es imposible nombrar a todos, pero no quisiera olvidarme de Adria G, Dani M, Nicola D, Anna J, Estanislao P, Jordi F, María P, Txell G, Albert N, Marco B, Andres P, Julia R, Víctor S, Olga M, Natalia C, Guillem, Laura C, Víctor B, Yoar C, Silvia S, Juan H, Francesca G, Isabel T, Arantxa S, Ester T, Rotman C, Alejandro S, Alejandro G, Manuela B,Alejandro B, Mar G, Enkhbayar D.....Tampoco me quería olvidar agradecer el apoyo logístico a Tere, Silvia, Ana y más recientemente a Mónica.

Además me gustaría agradecer el esfuerzo y la ayuda de Emilio R, Patricia C y Miguel L de la Facultad de Geologia de Barcelona (UB).

También quiero agradecer las revisiones y consejos de Teresa G y Josep F de la Agència Catalana de l'Aigua (ACA).

No podría haber terminado esta aventura sin la ayuda de mis chicas y chicos que me acompañaron durante este periplo o incluso algunos durante casi toda mi vida, tanto en Barcelona como por otras partes del mundo. Gracias por confiar en mí, por vuestro apoyo incondicional, vuestras sonrisas y vuestra amistad. Gracias Vane, Sandra, Anabel, Almu, Elena, Oski, Olgui, Bea, Pollo, Patri, Yoli, Caty, Ani, Anita, Luis, Sabi, Cris, Espe, Adela, Ana, Choni, Merche, Tania, Susi, Manu, Sonia, Luca, Umber, Alberrrrto y Moncho.

Quisiera dedicar esta tesis a mi familia, especialmente a mis padres que me han enseñado a ser curiosa, a disfrutar del conocimiento, a no rendirme nunca y sobre todo a vivir con alegría. Os quiero. También quisiera incluir a mi hermana Estrella, que siempre ha sabido que yo podía hacer esta tesis aún cuando yo no lo sabía. Gracias peque, por tu cariño y tu amistad.

Infine vorrei ringraziare il mio compagno di vita Marco Miozzo, per tutto il suo sostegno, la gentilezza e l'amore. Grazie mille, per avermi dato tanto in cambio di nulla, per avermi regalato un amore libero e vero... per essere stato al mio fianco. Volevo anche ringraziarti per avermi dato la possibilità di conoscere i tuoi cari, che mi hanno dato tanti consigli, especiamente a Paolo D.

Finalmente, me gustaría agradecer el apoyo del Ministerio de Ciencias e Innovación de España (proyectos HEROS: CGL2007-66748 y MEPONE: BIA2010-20244), al Ministerio de Industria de España (proyecto GEO-3D: PROFIT 2007-2009), a la Agència Catalana de l'Aigua (ACA) y a la Generalitat de Catalunya (Grup consolidat de recerca: Grup d'Hidrologia Subterrània, 2009-SGR-1057).

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# 1 INTRODUCTION

# 1.1 Aims and objectives

Sedimentary media (alluvial sediments, deltas, etc.) constitute important aquifers because of their high permeability, storage capacity, and interaction with surface water. In an urban environment, there is a considerable impact of human activity in terms of quality and quantity on groundwater (due to the sewerage system, the water supply network, etc.). Moreover, groundwater poses a problem for the development of infrastructure such as tunnels, basement crossings of large buildings, underground parking lots, etc (Vázquez- Suñè et al. 2005b, Pujades et al. 2011).

Groundwater models constitute an essential tool for a reliable water management in urban sedimentary media (Pokrajac 1999; Vázquez-Suñé et al. 2006; Carneiro and Carvalho 2010). These models allow us to conceptualize, identify and quantify the hydrogeological processes. They enable us to simulate various scenarios such as droughts, water resource exploitation, water quality evolution and interaction with civil works in terms of hydraulic and geomechanical behaviour of the ground.

The complex nature of the process that controls the sedimentary media often produces a highly heterogeneous distribution of hydrogeological parameters in aquifers. In this regard, some authors (Huggenberger and Aigner, 1999; Klingbeil et al., 1999; Heinz et al., 2003; Sharpe et al., 2003; Ezzy et al., 2006) have highlighted the importance of constraining the models of flow and transport of solutes to the sedimentological heterogeneities of the aquifer.

Nevertheless, defining the geological heterogeneities that control flow behaviour in sedimentary aquifers and especially, in those located under urbanised areas, is not easy. Outcrops, where they exist, are few and far between and data are sparse and are derived from diverse sources, making a suitable integration and management difficult.

In the last decades, advances in hydrocarbon exploitation and in hydrogeology have gone hand in hand with the development and implementation of new technologies. In this regard, the development of three-dimensional models of subsurface heterogeneity has proved to be an efficient tool for the management of reservoirs in geological scenarios (Matheron et al., 1987; Gundeso and Egeland, 1990; Stanley et al., 1990; Weber and van Geuns, 1990; Bryant and Flint, 1993; Krum and Johnson, 1993; Deutsch and Hewett, 1996; Dubrule and Damsleth, 2001) and for the management of water resources (Ross et al., 2005, Robins et al., 2005, Lelliot el al., 2006, Robins et al., 2008).

Apart from a detailed geological model, a comprehensive hydrogeological model must use all kinds of information available, i.e. hydrometeorological, geographical, hydrochemical, hydrogeological and environmental information, etc. Each field complements the interpretation of the rest of the fields. For instance, an appropriate hydrochemical analysis allows us to re-interpretate the geology, or a reliable geological analysis enable us to perform a proper parameterization of the study area that can be complemented with pumping tests.

The accomplishment of these tasks is not always straightforward because of a) the management and integration of a vast amount of time and spatial dependent data of different nature (e.g. hydrological, geological, etc), b) the homogenisation and harmonisation of data collected from diverse sources and gathered with different techniques (Rienzo et al 2008, Letoenau et al 2011), c) the communication and exchange of data of different formats (Wojda and Brouyere 2013), d) the management of data with varying quality standards and diverse temporal and spatial extensions and e) the need for integrating into the database the resulting interpretations and models derived from the raw data with the necessary documentation for re-use by third parties with different objectives (Refsgaard et al., 2010).

An optimum data management of this vast amount of spatial-temporal information cannot be readily handled without a comprehensive geospatial database that covers all the necessary concepts for dealing with a comprehensive groundwater characterisation. Besides, such a database should have at its disposal efficient tools for the gathering and the exploitation of raw data for their subsequent interpretations. Moreover, these interpretations should be correctly structured and included in the database for further cross-analyses (e.g. validation of a hydrogeological model with a geological model).

The use of the GIS-based approach proved to be a reliable method to implement groundwater database and to handle the interpretation and the analysis of the data taking into account most of the aforementioned aspects (e.g. Carrera-Hernandez et al 2008, Chesnaoux et al 2011).

As regards hydrogeology, GIS-based hydrogeological databases and tools have already been applied to a wide range of applications (e.g. Camp and Outlaw, 1993, Gogu et al., 2001, Strassberg, 2005; Gemitzi and Tolikas, 2006; Best and Lewis, 2010; Whittaker et al., 2012, Rhaman et al., 2012). Nevertheless, the following issues remain to be resolved: (1)the need for developing further tools that complement the existing tools implemented in the GIS platforms to perform a comprehensive 3D geological and hydrogeological analysis,(2) the scarcity of geospatial databases that are specially designed to store and manage the wide variety of hydrogeological spatial-temporal dependent data with the appropriate tools for retrieving additional information in the same GIS platform, and (3) the dearth of geospatial databases aimed at integrating the resulting interpretations and models derived from raw data with the documentation for re-use.

In the light of the foregoing, the first aim of this thesis was to develop a reliable GIS-based platform composed of a geospatial database and a set of GIS-tools that arrange all the available data into a coherent structure and provide support for its proper management,

analysis and interpretation. Furthermore, this platform facilitates the pre- and post-processing of the hydrogeological data for modelling.

The second aim of this thesis is to implement this modelling platform in the urban area of Barcelona (NE, Spain) to structure all the available data and set up a working framework of groundwater resources in terms of quantity and quality for this area.

The urban area of Barcelona with over 3 million inhabitants is located on the Mediterranean coast in the NE of the Iberian Peninsula. Geologically, this area consists of a coastal plain limited by two deltaic formations and a higher area, the Catalan Coastal Ranges.

The sedimentary aquifers have been exploited for domestic and industrial use in recent decades, which has seriously compromised the quantity and quality of the groundwater resources of the study area. Moreover, this region has an active underground infrastructure, which also poses a threat to the quantity and quality of groundwater resources.

# 1.2 Thesis outline

This thesis consists of four principal chapters (chapters 2 to 5) in addition to the introduction (chapter 1), general conclusions (chapter 6) and reference list (chapter 7). The main chapters are based on papers that have been published, accepted or submitted to international journals. The references to the papers are contained in a footnote at the beginning of each chapter. One annex lists the articles and reports concerning the development of this thesis and the participations in scientific congresses and seminaries.

Chapter 2 highlights the need for developing a software platform in a GIS-environment that combines in a unique platform a geospatial database (HYDOR) and three families of utilities aimed at facilitating: hydrochemical data interpretation (QUIMET), 3D geological analyses and modelling (HEROS) and other hydrogeological analyses (HYYH). In this chapter, we focus on describing the last set of tools (HYYH) and the database model of HYDOR. Section 2.2 provides a review of the general advances made in the development of the database and tools. Moreover, this chapter presents the implementation of this data model in the urban area of Barcelona (NE, Spain).

Chapter 3 describes the methodology and instruments created for generating 3D geological models using the set of geological analysis tools (HEROS). The second section of this chapter undertakes a critical review of commercial and research instruments that assist the creation of 3D geological models with special emphasis on the GIS-based software platforms. This chapter also includes an application of these tools in a study area located in Barcelona.

Chapter 4 gives an overview of the Hydrochemical Analysis tools (QUIMET) and offers an example using data from a coastal area in the urban area of Barcelona (Badalona, Spain). This chapter also includes an evaluation of existing software tools to perform hydrochemical analyses to account for the work presented.

Chapter 5 focuses on the application side of the GIS-based platform and presents a sequence stratigraphic-based 3D geological model of the Quaternary Besos Delta (urban area of Barcelona, Spain), which was used to constrain the distribution of hydraulic parameters and thus to obtain a consistent hydrogeological model of the Delta.

Chapter 6 contains the summary of the main conclusions of the thesis and chapter 7 lists the references.

# 2 GIS-BASED HYDROGEOLOGICAL DATABASE AND ANALYSIS TOOLS

# 2.1 Introduction

Groundwater represents an important source of water. Evaluating and predicting its availability and accessibility is therefore one of the main tasks in Integrated Water Resources Management (IWRM) (Barthel et al., 2008).

In an IWRM framework, the development of hydrogeological models is required to predict the impact of different land and water management. Moreover, all data employed in modelling should be easily accessible to decision makers and modelers (Carrera and Gaskin, 2008).

Models are a representation of the reality (Cunge, 2003), but reality is elusive. A comprehensive hydrogeological model demands the use of a wide variety of information, i.e. geological, hydrometeorological, geographical, hydrochemical, hydrogeological and environmental, etc. Each field complements the interpretation of the rest of the fields. For instance, a proper hydrochemical analysis allows us to re-interpret the geology and a reliable geological analysis enables us to perform a proper parameterization of the study area that can be complemented with pumping tests.

In practice, this interpretation process may encounter a number of difficulties: a) the management and integration of a vast amount of time and spatial dependent data of all kinds( e.g. hydrological, geological, etc), b) the homogenisation and harmonisation of data collected from diverse sources and gathered with different techniques (Rienzo et al., 2008;Létourneau et al.,2011), c) the communication and exchange of data of different formats (Wojda and Brouyere, 2013), d) the management of data with varying quality standards and diverse temporal and spatial extent, e) the need for handling and retrieving geological and hydrogeological data for representing the heterogeneity of the aquifer systems in the three dimensions of space (e.g. Ross et al., 2005; Robins et al., 2008; Velasco et al.,2012a; Velasco et al., 2012b) and f) the necessity of integrating into the database the resulting interpretations and models derived from the raw data with the necessary documentation for use by third parties for different objectives (Refsgaard et al.,2010).

This chapter is based on a submitted paper: Velasco, V., Criollo, R., Vázquez-Suñè, E., Alcaraz, M., Serrano, A., Garcia-Gil, A., Gogu, R., 2013, submitted. GIS-based hydrogeological database and analysis tools. Environmental Modelling & Software.

An optimum data management of this vast amount of spatial-temporal information cannot be readily handled without a comprehensive geospatial database that covers all the necessary concepts for dealing with an entire groundwater characterisation.

Besides, such a database should have at its disposal efficient tools to gather and exploit the raw data for further interpretations. Moreover, these interpretations should be correctly structured and included in the database for subsequent cross-analyses (e.g., validation of a hydrogeological model with a geological model).

The use of a GIS-based approach has proved to be a reliable method to implement groundwater databases and to interpret and analyse the data taking into account most of the aforementioned aspects (e.g. Strassberg et al., 2007; Sanz et al., 2009; Chesnaoux et al., 2011).

The use of GIS improves the visualisation and the editing of data through the simultaneous display of different layers and more advanced 3D views. These applications increase the integration of quantitative and qualitative data and enable straightforward consultation, search, and retrieval of portions of information provided by different sources of spatial data (Descamps et al., 2005). Moreover, the combination of databases and GIS software packages not only constitutes a valuable support for the creation of data structure for the interpreted data but also maintains a simple interface with the user, obviating the need to know the complexity of the data model.

As regards hydrogeology, GIS-based hydrogeological databases and tools have already been applied to a wide variety of applications (e.g. Gogu et al., 2001; Strager et al., 2010; Rhaman et al., 2012). However, because of the complexity and large number of methodologies involved in groundwater characterisation, some procedures still lack refinements (e.g. the possibility of performing a hydraulic parameterisation from detailed geological analyses with the support of tools to manage hydraulic test results in the same scenario).

In this context, we developed a novel GIS-based platform. It is composed of a geospatial database and a set of GIS tools that arrange all the available data into a coherent structure and provide support for their proper management, analyses and interpretations.

In detail, these GIS tools provide three families of utilities aimed at facilitating: hydrochemical data interpretation (QUIMET; Velasco et al., 2013a), 3D geological analysis and modelisation (HEROS; Velasco et al., 2012b) and other hydrogeological analyses (HYYH, presented in this chapter).

The aim of the present chapter is twofold. First, we present the aforementioned GIS based platform by focusing on the geospatial database and on the tools for hydrogeological analysis (HYYH). Secondly, we discuss the implementation of this model in the metropolitan area of Barcelona (NE Spain) and the evaluation of this working framework of groundwater resources. It should be noted that the framework presented can be applied to other study areas.

Section 1.1 of the present chapter is constituted by the introduction. Section 2.2 provides a review of the existing hydrogeological database models with their corresponding tools. Section 2.3 contains a detailed discussion of the novel GIS based platform. Section 2.4 focuses on the application of this platform to the metropolitan area of Barcelona. Finally, the main conclusions arising from the application of the software together with its advantages, limitations and possible further developments are presented in section 2.5.

# 2.2 Background

This section reviews some existing projects that inspired the design of the database and the development of the tools to exploit the information presented here. The review begins by examining some existing groundwater data models paying particular attention to the projects that have also developed tools to exploit the available data in a GIS environment.

In the early nineties, Camp and Outlaw, 1993 developed a complete well log database based on information obtained from driller's logs and electrical geophysical logs. Additionally, a procedure for constructing geological profiles for providing geometric data for groundwater flow and contaminant transport models has also been created using ARC/INFO (ESRI, 1993).

Some years later, Gogu et al., 2001 developed one of the first reliable GIS-based hydrogeological databases for the Walloon region in Belgium. It is a GIS-based database that offers facilities for groundwater-vulnerability analysis and hydrogeological modelling. This database manages efficiently geological, hydrochemical, climatological and further hydrogeological information using ARC/INFO (ESRI, 1997). Furthermore, it includes a set of tools to perform spatial-temporal queries of some of the data included in the database such as hydraulic head or pumping well allocations.

Thereafter, Cabalska et al., 2005 developed a functional system composed of GIS-tools that facilitate data consultation and retrieval of a complete database which integrates several existing databases in the Polish Geological Institute (PGI, 2013). The database includes a variety of hydrogeological, hydrochemical, geological and meteorological information. The GIS-tools, developed in the *Geomedia Pro platform*, enable the graphical representation of some data integrated into the database, their spatial analysis and the generation of hydrogeological cross-sections.

Despite these advances, there continues to be a need for other tools to perform and store detailed 3D characterisation of the study area and also for tools to facilitate further hydrogeological analyses.

Strassberg, 2005 overcame this drawback by developing a GIS-based data model (ArcHydro Groundwater model) to represent groundwater systems that expand the existing ArcHydro surface data model (Maidment, 2002). The data model (implemented within ArcGIS; ESRI, 2004) was designed to include raster, feature-class and tables to represent aquifers,

wells, temporal and vertical information recorded along boreholes. In addition to the geodatabase, two sets of tools have been developed to help users create data structures within the data model. The first set of tools operates within ArcScene and supports the creation and the storage of 3D objects such as hydrostatigraphy, cross-sections and volumetric objects. The second set of tools facilitates the generation of 2D/3D modelling elements such as cells and models. Besides, the database structure enables the generation of SQL queries to map time series in 2D and 3D.

This framework provides efficient tools for the management and interpretation of hydrogeological data. Nevertheless, further procedures may be improved especially for the management and retrieval of detailed geological data and hydrogeological experimental tests.

Whiteaker et al., 2012 facilitate the management and interpretation of geological data integrating 2D cross-sections and 3D representations into the site characterizations in ArcGIS by using the presented ArcHydro Groundwater model.

Chesnaux et al., 2011 present an effective methodology to build a comprehensive database through a combination of Relational Database management Systems (RDBMS), ArcGIS and the aforementioned ArcHydro Groundwater Tools. Additionally, these authors introduce a process for increasing the efficiency of the geodatabase thanks to instruments developed for data quality control. The database includes a wide variety of hydrogeological data; among them results of experimental tests such as pumping tests, specific capacity tests, grain size analysis and prediction of the hydraulic conductivity of the aquifers.

Further advances in the storage of field test observations and interpretations can be found in the H+ database (de Dreuzy et al., 2006), which provides an interface between experimentalists and modellers. This database structure enables us to store a large number of data and data types collected for a given site or multi-site network. It is designed to manage a broad range of information that incorporates both routine monitoring of point collections and experimentally derived data from several site collections. It is enriched with a fully functional web-based user interface; nevertheless further tools for interpretation and visualization of data are still needed.In addition, the generic structure proposed as a template does not describe a conceptual data model for specific hydraulic tests (Wojda et al., 2010).

Wojda and Brouyere, 2013 present a complete Hydrogeological data model (H<sup>g</sup><sub>2</sub>0), highlighting specialised hydrogeological field experiments such as hydraulic and tracer tests. This database has been implemented in the Web2GIS web (Laplanche, 2006) which offers tools for model conception, database implementation and visualisation. In addition, the data model has also been implemented in the ArcGIS desktop which provides a wide range of tools for analysis, retrieval and interpretation. However, further specific tools are still needed for the retrieval and storage of 3D geological and hydrogeological properties and for interpreting other hydrogeological data (e.g. specific hydrochemical diagrams).

In order to facilitate data exchange, this model complies with the recommendations of the European Geospatial Information Group (Vogt, 2002) and follows the guidelines of the International Organisation for Standardisation Technical Committee 211 (ISO/TC211) and the Open Geospatial Consortium (OGC). Finally, it proposes a simplified approach based on the Observations&Measurements standard (OGC, 2003; OGC, 2006; OGC, 2007) to manage hydrogeological data such as time series of piezometric heads and field measurements and observations.

In addition to the aforementioned models and in line with Wojda and Brouyere, 2013, International Standards and on-going projects concerning encoding and exchange of geospatial information were also taken into account to develop the hydrogeological data model presented here. This includes the Geological data specifications of the European Directive INSPIRE (INSPIRE, 2013), the ONEGeology project (OneGeology, 2013), the Australian National Groundwater Data Transfer Standard (1999), the Common Implementation Strategy for the Water framework directive (2000/60/EC) (WFD, 2007), GeoSciML (Sen and Duffy, 2005), Water ML.2.0 (OGC, 2012) and the Observations&Measuremens standard (INSPIRE, 2011).

# 2.3 Proposed GIS-based platform

In the light of the aforementioned discussion, a new hydrogeological database model was developed together with a set of tools to improve the visualisation, processing and interpretation of the hydrogeological data constituting a GIS-based platform.

This software platform was designed bearing in mind the different tools and methodologies that water managers use to evaluate, integrate and analyse the wide range of information for the construction of a hydrogeological model. Consequently, the following requirements were taken into consideration to design the software platform:

- I. Management and storage of spatial features and time dependent data on a geospatial database. The design of the database should support:
  - I.1. The representation of different spatial-temporal scales of groundwater systems.
- I.2.The integration of different types of information (e.g. groundwater, hydrometoerological, hydrological).
  - I.3. The possibility of the standardisation and harmonisation of data.
  - I.4. The integration of interpreted data.
  - I.5. The extraction of archived groundwater data for use with external software.
  - II. Data processing and analysis using:

- II.1. Instruments to perform accurate geological analysis and creation of 3D models: a) specific instruments to perform accurate stratigraphic analysis, visualisation of stratigraphic columns and generation of cross-sections b) tools to generate 3D surfaces of isopach and isobath maps and c) tools to generate fence-diagrams.
- II.2. Tools to facilitate the hydrochemical analysis by using quality controls, computation methods, statistical analysis and traditional graphical analysis techniques (e.g. Piper, Stiff and salinity diagrams).
- II.3. Instruments to query and represent other hydrogeological data such as groundwater level, aquifer tests and well abstractions or injections.
- II.4. Tools that enable the hydraulic parameterisation by using calculations based on the textural characteristics of the terrain and based on hydraulic test interpretations (i.e. pumping and tracer tests).
- II.5. GIS environment which provides: a) different interpolation tools to estimate/validate the distribution of different parameters such as hydrogeological, hydrochemical, petrophysics, hydrological, hydrometeorological properties, b) Index overlay techniques and c) a wide range of in built utilities for further analysis (e.g. Spatial Analysis Tools, Geostatistical Tools, Mapping tools, etc).
  - III. Native interaction with external software for further analysis using:
- III.1. Geostatistical software packages such as SGems (Remy, 2009) or GSLIB code (Deutch and Journal, 1998).
- III.2. Software packages especially designed to characterise the recharge (e.g. EASYBAL (Serrano et al., 2013; GHS, 2013a).
- III.3. Codes to facilitate the hydraulic tests interpretations such as EPHEBO/MariaJ code (GHS, 2013b)
  - III.4. Pre-processor packages to generate 3D mesh such as GID (CIMNE, 2013).
- III.5. Groundwater modelling packages such as TRANSIN (Medina and Carrera, 2003, Medina et al., 2000) and VisualTransin (GHS, 2013d).
- III.6. Hydrogeochemical modelling packages such as PHREEQC (Parkhurst and Appelo, 2013), NETPATH (Plummer et al., 1994) and MIX (Carrera et al., 2004; Serrano et al., 2013; GHS, 2013c).
  - IV. Post-processing tools to facilitate the integration of the results obtained from analysing and interpreting the hydrogeological data included in the database, in the same GIS environment or in an external platform.

### 2.3.1 HYDOR database

The geospatial database HYDOR represents geospatial information based on the Personal Geodatabase structure provided by ArcGIS (ESRI, 2012).

The database design enables the user to extend the scheme if necessary. This framework offers a very good interface for geospatial data management and the possibility to exchange geospatial data through XML which extends its interoperability (Wojda and Brouyere, 2013). Moreover, although the data model of the hydrogeological database described here was implemented within ArcGIS, most of these concepts are sufficiently flexible to enable implementation into other platforms.

The first step in the development of the database was the creation of a conceptual model of the required information. The data model of HYDOR is conceptualized in 8 main components: Geology (e.g., boreholes lithological description, stratigraphic units, depth to bedrock), Geophysics (e.g. diagraphies), Hydrogeology (e.g. well descriptions, springs, head measurements, extraction measurements, hydrochemical measurements), Hydrology (e.g. rivers, lakes, sea), Hydrometeorology (e.g. precipitation, temperature), Environment (e.g. protection zones),Regional Geography (e.g. topography, cities) and Water Management Administration (e.g. River Basin Districts).

Each of these components is represented in the geospatial database by a feature dataset composed of a group of feature classes (points, lines and polygons). In addition to feature classes, several tables are used to represent and store the attributes of the features and the observations and measurements obtained. Other information such as the digital elevation model of the terrain and boundaries of geological units are stored in raster catalogues. Relationships within the data model link feature classes and tables and establish logical connections between data layers (See Fig.2.1).

[Chapter 2: GIS-based hydrogeological database and analysis tools]

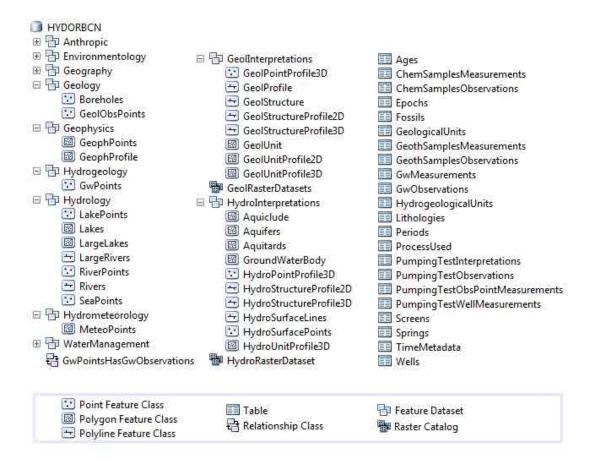


Figure 2.1. Simplified ArcCatalog view of the HYDOR database model.

# 2.3.1.1 Description of data contained

This section describes the most important or innovative elements of the HYDOR database, highlighting the most used aspects in groundwater characterisation. Other datasets (*Interpreted dataset*) containing interpretations and calculations obtained from these data are shown in section 2.3.3. Finally, the reader is referred to Velasco et al 2012b and Velasco et al, 2013a for further details about geological and hydrochemical components of the database.

### I. Geological components

The database structure allows storage of accurate geological data that can be generalised and subsequently up-scaled. The geological dataset includes data related to boreholes, outcrops, interpretations and definitions of geological units/subunits, etc. Furthermore, the geological data are linked to other datasets such as geophysical, hydrochemical and hydrogeological components, which complements the geological interpretation. The most relevant components of this dataset are described below.

### I.1. Boreholes

One of the main components of the geological dataset is **Boreholes**, which is a point feature class describing borehole locations and attributes. **Boreholes** provide information that is used to characterise the subsurface. The observations recorded within a borehole such as its lithological (**Lithology**), paleontological (**Fossils**), chronological (**Age, Period, Epoch**), geotechnical (**GeotechnicalObservations&Measurements**) characteristics are stored in different tables linked to the **Boreholes** feature class. These observations are expressed as intervals that correspond to different depths along the borehole.

### I.2. GeolObservationsPoints

Although the main source of geological information in an urban area is provided by the boreholes, other geological observation points (**GeolObservationPoints**) such as pits or outcrops were included in the database. As with the **Boreholes** feature class, this entity is linked to the same tables for storing its geological and geotechnical characteristics (i.e. **Lithology, Fossils**, etc.).

### I.3. GeologicalUnits/SubUnits

These tables store the different properties of the identified geological units, such as type (e.g. biostratigraphic, allostratigraphic,) and general composition (e.g. dolomitic, sulphate, etc.). In line with the definition of the *Geological Units* class established by INSPIRE, 2013 these tables are conceptual entities and enable a single real world geological unit to have multiple map representations (2D, 3D, sections, etc.). The aforementioned representations depend on the available data and on the objectives of the project (e.g. regional, local-site study). In order to maintain the difference between raw data and interpreted data, all the spatial representations of the **GeologicalUnit/Subunits** are stored separately in the *Interpreted dataset* (section 2.3.3).

The definition of the boundaries (top and bottom) of the different **GeologicalUnits/Subunits** for each borehole or geological observation point is stored in tables **BoreholeGeolUnits/SubUnits** and **GeoObsPointGeolUnits/Subunits**.

# I.4. GeologicalStructures

The table **GeologicalStructures** was designed to store and represent the different properties od the geological structures such as faults and contact surfaces identified by direct observation (over the terrain, orthophotos, etc) or by further interpretation of the geological data (e.g. borehole correlation). As with the **GeologicalUnits**, this table contains properties that enable a single real world geological structure to have multiple representations in 2D or 3D which are also stored in the *Interpreted dataset* (section 2.3.3).

# II. <u>Hydrogeological components</u>

The hydrogeological dataset of the data model includes the representation of hydrogeological units, groundwater bodies and aquifer systems in a number of spatial forms. Moreover, this dataset contains features class and different attribute tables to describe manmade or natural objects where interaction occurs within the hydrogeological system. Finally, a wide range of hydrogeological spatial-temporal dependent data such as piezometric heads or hydrochemical measurements among others can be easily managed within the database (see figure 2.2, 2.3 and 2.4).

# II.1. Hydrogeological Units

The **HydrogeologicalUnits** table stores the conceptual description and attributes of the hydrogeological units identified. A hydrogeological unit is a part of the terrain with distinct parameters for water storage and conduction. There are 3 main subclasses of hydrogeological units: Aquifer, Aquitard and Aquiclude.

The design of these feature classes are essentially based on the recommendations given by the INSPIRE, 2013. For instance, the **Aquifers** feature class contains all properties of the aquifer systems such as aquifer media type (e.g. porous, fractured, etc), aquifer type (e.g. confined, unconfined, etc), hydrogeochemical rock type to define the natural hydrogeochemical condition (e.g. siliciclastic, carbonatic, etc), vulnerability to pollution, mean storativity coefficient and mean permeability.

Additionally, the table **AquiferSystems** represents a collection of aquifers and/or aquitards which together constitute the environment of groundwater - "communicating vessels" that are filled or can be filled with groundwater i.e. a **GroundWaterBody**.

These features have different spatial representations in 2D and 3D as the **GeologicalUnits** and they are also stored in the *Interpreted dataset* (section 2.3.3). The definition of the boundaries of the different hydrogeological units identified for each borehole (**Boreholes**) or for each geological observation point (**GeolObsPoints**) is stored in the tables **BoreholeHydroUnits** and **GeolObsPointHydroUnits**.

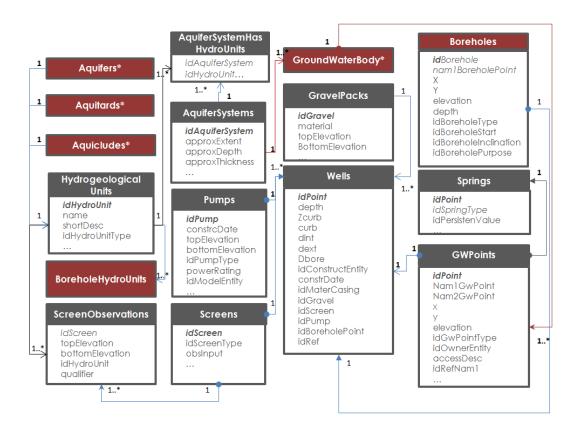


Figure 2.2. Simplified conceptual diagram representing some of the hydrogeological content of the HYDOR geospatial database including HydrogeologicalUnits, GwPoints and the different tables that describe the Wells properties. The 1 and 1..\* represents the cardinality of the relatioinships between tables.

# II.2. GroundwaterBody

This polygon feature class represents a distinct volume of groundwater within an aquifer or aquifer system, which is hydraulically isolated from nearby groundwater bodies (INSPIRE, 2013). This feature contains general information of the groundwater body such as the water type (e.g. fresh water, saline water, etc) and the degree of change as a result of human activity (e.g. natural, modified, slighty modified, ect). **GroundWaterBody** is linked to a number of entities such as **AquiferSystems** and **WFDGroundWaterBody**, which is a management unit within the Water Framework Directive (WFD).

Besides, global piezometric characterisation of the groundwater body for different time intervals is stored in the associated table **PiezometricState**. Likewise, **PiezometricState** is related to the **HydrogeologicalSurfaces** (representing the geometry of any hydrogeological surface based on hydrogeological measurements in a group of wells) which is stored in the *Interpreted dataset* (see section 2.3.3).

### II.3. GwPoints

This point feature class is focused on representing punctual man-made (e.g. well, mines) or natural objects (e.g. springs, geysers) where interactions occur within the hydrogeological system. The main attributes of this *GwPoints* are the geographical coordinates, the description of the different names used to identify these points of information (potential different sources of data), the type of groundwater point (well, piezometer, spring, etc.), point accessibility, related groundwater body and other administrative information. Moreover, information specific for each groundwater point type is stored in different tables. The most common *GwPoints* types in use are:

### • Wells

The table **Wells** stores specific properties of wells and piezometers such as activity (e.g. monitoring, dewatering, disposal, recharge, etc.), depth, status, dimensions of the curb, related borehole, etc. In order to complete the description of the wells, different tables were defined: a) **Pumps**, which stores the properties of the pump of the wells should one exist, b) **Gravels**, which describes the gravel pack properties and c) **Screens**, which describes the screen type (e.g. continuous-slot, slotted plastic pipe, etc) and d) **ScreenObservations**, which stores the intervals screened. The latter, also establishes for each given screened interval, the link of the well to the hydrogeological unit which is screened .Thus, a well can be screened in diverse hydrogeological units whereas a hydrogeological unit is screened by different wells.

### Springs

The table **Springs** stores specific properties of springs, such as spring type or water persistence (e.g. intermittent, seasonal, etc.).

# II.4.GwObservations&Measurements

To manage hydrogeological data observed at a given groundwater point (**GwPoints**) such as time series of head measurements, or rate and volume of abstraction or recharge, the tables **GwPointsObservations** and **GwPointsMeasurements** were designed (see Fig.2.3). Several tables containing further details such as those related to the temporal measurements (**TimeMetadata**) and the process used to carry out the observation (**ProcessUsed**) are linked to these tables. A code list of hydrogeological measurements with its corresponding units (**LibGwParameters**) was also developed.

In addition, other vertical measurements are considered in the **GwVerticalMeasurements** table (as Strassberg, 2005).

This dataset was designed taking into account the guidelines provided by the Observations and Measurements (O&M) and WaterML 2.0 standards. As a result, a modification that was easy to implement in a GIS-managed database was made.

# II.5. ChemSamplesObservations&Measurements

These tables (**ChemSampleObservations** and **ChemSampleMeasurements**) contain information about the hydrochemical measurements realized in both groundwater points and surface-water points. Detailed information about this dataset and its related tables (e.g. **LibChemParmLab, LibNormative**) can be seen in Velasco et al., 2013a.

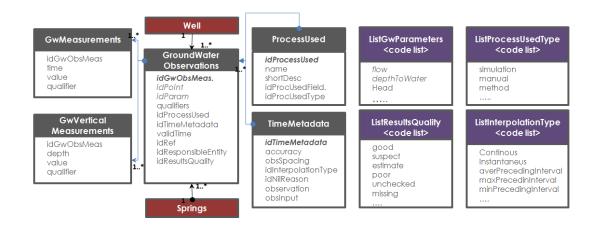


Figure 2.3. Simplified conceptual diagram representing some of the tables that include the GwObservations& measurements observed in the GwPoints. The 1 and 1..\* represents the cardinality of the relationships between tables.

# II.6. HydraulicTests

Hydraulic tests (e.g. pumping tests, tracer tests) are commonly used by hydrogeologists to determine a wide variety of hydraulic properties of an aquifer system. Normally, this type of field-tests generate a large amount of complex spatio-temporal dependent data that are difficult to manipulate for subsequent analysis and interpretation. To overcome these difficulties, a dataset was generated to store the majority of the existing types of pumping and tracer tests.

According to Wojda and Brouyere, 2013, the information required for a generic analysis of aquifer tests consists in: a) the description of the experimental setup, b) observations retrieved at different locations in space and in time during the experiment and c) the interpretation of these observations with its methodological description.

Apart from these conceptual issues, the design of this dataset was performed taking into account the following requirements: a) it should be easy to fill-up and query (i.e. the name of the attributes should be representative and the entry protocol should be clear for the water managers), b) the measurements and observations obtained in a hydraulic test (e.g. water extraction/injection, drawdown profiles, or chemical measurements of the tracer) should be stored separately from the general **GwObservations&Measurements** to avoid

misunderstanding in a general temporal-spatial query of the groundwater points and c) the design of the tables should support a wide variety of workflows for tracer and pumping tests.

This dataset is composed of the following tables (see Fig. 2.4.):

#### Tests

This table contains general information of the hydraulic test such as name, campaign, date, responsible, type of test (related to **TestType**) and study area (related to **StudyArea**). The rest of the experimental setup information such as the wells and piezometers involved in the experiments or the characteristics of the tracers injected are stored in different tables linked to this one. Additionally, the observations and measurements retrieved during the tests and the interpretations obtained from these observations are stored in separated tables.

# • PumpingTestWellSpecification

This table stores the information about the pumping period and other incidents of the pumping device occurring at the wells during the pumping test.

# • PumpingTestObservations&Measurements tables

As with the GwObservation&Measurements, these tables were designed following the general guidelines of O&M standards with some specifications for improving the introduction, management and query of the data related to pumping tests. Consequently, PumpingTestObservations table includes the feature of interest (well or observation point), the characteristics of the time-series (TimeMetadata) of the measurements performed during the test (e.g. flow profile or drawdown) and other important characteristics of the experiments such as the process and the device used in the experiments (ProcessUsed). The PumpingTestWellMeasurements table stores the information retrieved in the well (flow and accumulative volume) where the pumping occurs whereas the PumpingTestObsPointsMeasurements table stores the information of the drawdown or head measurements performed at the monitoring points. The design of the structure of the database considers that for a given pumping test various wells can extract/inject water simultaneously or at different periods of time. Likewise, these wells can act as monitoring points and vice versa.

Finally, the different parameters interpreted from these experiments as well as other details about the methodology are stored in the **PumpingTestInterpretations** table. For a given experiment, different interpretations can be obtained depending on the methodology used.

#### • TracerTestObservations&Measurements

The observations retrieved in a tracer tests is stored in this group of tables. The **TracerTestPointInjection** table stores and manages the information related to the injection

procedure such as injection point, process used, injected volume, type (punctual or continuous) and the characteristics for each tracer used (TracerTestChemInjections) together with the date and duration of the injection.

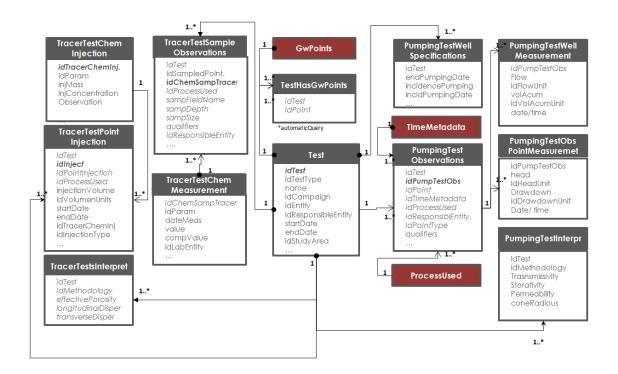


Figure 2.4. Simplified conceptual diagram representing the most of the tables involved in the storage and management of the data related with the hydraulic tests. The 1 and 1..\* represents the cardinality of the relationships between tables.

The *TracerTestSampleObservations* table stores the information of the measurements made at each sampling point. This sample is stratified in accordance with, sampling data, sample name, sample size and depth .Thereafter, each sample analysis is stored in accordance with sampling data analysis, parameter, value and units of measurement in the *TracerTestChemMeasurements* table.

The **TracerTestsCountinousObservations** and **TracerTestContinousMeasurements** tables include information of the tracer measurements made by continuous tracer test instrumentation.

Finally, the different parameters interpreted from these experiments as well as other data about the methodology are stored in the **TracerTestInterpretations** table.

# III. Geophysical components

This dataset was designed to store commonly used geophysical measurements made in groundwater characterisation. This dataset includes two main feature-classes that represent the location and projected geometry of geophysical activity: **GeophPoints** and **GeophProfiles**.

#### III.1. Geophysical profiles

This line feature-class (**GeophProfiles**) was designed to represent the location and the main attributes of the geophysical measurements spatially referenced to a projected line (e.g. seismic lines).

#### III.2.Geophysical points

It is a point feature-class (**GeophPoints**) that indicates those geophysical measurements spatially represented as points, such as diagraphy.

#### III.3. Geophysical observations&measurements

The **GeophysicalObservations** table stores the main characteristics of the geophysical measurements performed in the **GeophPoints** such as the experimental data set (related to **Process Used**). The resulting values are stored in the linked **GeopysicalVerticalMeasurements** table.

# IV. <u>Hydrological components</u>

Traditionally, management water resources have been focused on surface water or ground water as if they were separated entities, but practically all surface water features (e.g. rivers, lakes, etc) interact with groundwater (Winter et al., 1999).

The general scheme includes spatial elements that take into account the WISE Reference GIS dataset (WFD, 2009). The WISE Reference GIS datasets have been created using detailed digital spatial data supplied by Member States and other sources, generalised for visualisation and assessment of geo-referenced data across Europe.

In addition, other datasets and feature-classes were specifically defined to include different observations for a complete groundwater characterisation and for describing the relationship of groundwater and surface water.

A number of approaches facilitating the estimation of the flow between surface water and groundwater have been developed. The most of these approaches are dependent on the head difference between the surface water and the aquifer, the spatial dimension of the surface water and the hydraulic conductivity of the surface water body bed (Strassberg, 2005).

#### IV.1. Rivers

The main aim of this line feature-class (**Rivers**) is to represent the rivers or a segment of a river included in a given hydrogeological analysis. Therefore, apart from the spatial dimension of the surface water this feature class includes attributes of the surface water bed such as hydraulic conductivity or thickness of its bed layer. This feature class can be related to the rivers or to the river basin defined in accordance with the *WISE reference GIS dataset* (e.g. **LargeRiver**, **RiverBasinDistrict**).

#### IV.2. Lakes

As with **Rivers**, this polygon feature-class (**Lakes**) represents the lakes or portion of a lake included in a given hydrogeological analysis and contains the information required for an aquifer-lake relationship. Finally, this feature can also be related to **Lakes** defined by the *WISE* reference GIS dataset (e.g. **LargeLakes**, **MainLakes**).

#### IV.3. Lake/River/SeaPoints

These feature classes represent point features located in a **Lake**, **River** or **SeaPoint** where an observation has been made. Apart from the spatial information of these observation points, these feature classes contain information on the lake or river point type (monitoring station, sampling site), accessibility, etc.

#### IV.4. Surface water Observations&Measurements

This dataset follows the same system and structure as GwObservations&Measurements described Consequently, above. these tables (SurfWaterObservations and SurfWaterMeasurements) store a wide variety of hydrological data such as water flow and water level measurements together with information about the gauging stations or the sampling points.

# V. <u>Hydrometeorological components</u>

The location and attributes of a meteorological station is stored in the point feature class termed **MeterologicalStation**. The different observations and measurements obtained (e.g temperature, precipitation) are linked to this table and follow the same system and structure as the **GwObservations&Measurements** or the **SurfWaterObservations&Measurements**.

#### 2.3.1.2 Entering the data

As for data insertion, the management system of the geodatabase enables the possibility of importing information coming from different formats such as spatial or non-spatial databases or spreadsheets. Furthermore, different forms are available for "one to one"

or "massive data". Digital data (other database or spreadsheets) can be transferred to the geospatial database through the use of intermediate conversion tables or existing wizards of ArcGIS following an entry protocol. If the data are hand written, they should be introduced manually using assisted menus.

In order to avoid errors when introducing data and in order to improve the harmonisation and the analysis of the hydrogeological data, data control procedures were developed. For instance, several permissible value lists were introduced to facilitate the encoding following recommendations of existing standards and directives (e.g. INSPIRE, OneGeology, etc.). In addition, some classes and their attributes provided by those standards were imported to guarantee future data exchanges

Finally, a protocol to reference the original source of information (e.g. maps, technical reports, scientific journal, files, etc) was also established in order to allow the user to consult the source documentation.

# 2.3.1.3 Querying the data

To facilitate data retrieval and expedite the spatial analysis process of the hydrogeological data, a series of GIS-based tools and other specific query forms were developed and will be discussed below. Other spatial and non-spatial queries may also be generated from the geodatabase by using the inherent capabilities of ArcGIS and/or by using the standardised MS Access query builder. Interested readers are referred to further documentation of ArcGIS and MS Access in order to perform other queries.

# 2.3.2 GIS-based tools

This set of analysis tools was developed as an extension of the ArcMap environment (ArcGIS; ESRI 2010). They were created with ArcObjects, which is a developer kit for ArcGIS, based on Component Object Model (COM), and programmed in Visual Basic using the Visual Studio (Microsoft) environment (see Velasco et al., 2012b, Velasco et al., 2013a).

They were set up to manage, visualise, analyse, interpret and pre and post process the data stored in the spatial database. This set of tools is separated into three main modules represented by different toolbars integrated into ArcMap termed HEROS, QUIMET and HYYH.

# 2.3.2.1 Geological Analysis Tools (HEROS):

The first module (HEROS) allows the user to exploit the geological data stored in the database to facilitate the geological interpretation. Detailed stratigraphic columns of the selected boreholes can be generated using customized queries by using the *Borehole Diagram Instruments*. The automatic creation of a geological profile is possible by displaying the borehole lithological columns, the geophysical and geotechnical field-test results and the defined stratigraphic units by using the different utilities of the *Stratigraphic cross-section* 

correlation tools. Thus, an interactive analysis environment is created, where the user is able to analyse and to define the possible existing correlation surfaces, units, and faults. These spatial elements can then be converted within a 3D environment and can be visualized in the same ArcGIS platform (ArcScene) or easily exported to external platforms such as GID for further analyses. Finally, hydraulic conductivity can be computed automatically (with the *Tools for the hydraulic conductivity estimation*) based on textural properties of each lithological interval defined in the boreholes or for each unit defined (for further information see Velasco et al., 2012b).

# 2.3.2.2 Hydrochemical Analysis Tools (QUIMET)

The second module (QUIMET) is composed of a set of instruments for analysis that cover a wide range of methodologies for querying, interpreting and comparing groundwater quality parameters (Velasco et al., 2013a). The Spatial QUIMET tools include chemical timeseries analyses, ionic balance calculations, correlation of chemical parameters, and calculations of various common hydrogeochemical diagrams (e.g. Schöeller-Berkaloff, Piper, Stiff). The GIS platform allows us to generate maps representing the spatial distribution of several hydrogeochemical parameters and of the aforementioned specific hydrogeochemical diagrams. Moreover, it is also possible using Statistical QUIMET Tools, to perform a complete statistical analysis of the data including descriptive statistic, univariate and bivariate analysis, the generation of correlation matrices of several components, calculation of correlation graphics, etc.

Finally, other instruments enable us to automatically retrieve the information necessary to perform subsequent calculations with external software such as MIX code or EASYQUIM (GHS, 2013b).

## 2.3.2.3 Hydrogeological Analysis Tools (HYYH)

Finally, the most recent module (HYYH) was designed to analyse and visualise different hydrogeological measurements and the results of the hydraulic field tests. A detailed description of the different commands and results that offers this set of analysis tools is presented below (see Fig.2.5). We are currently working on improving and extending the functionabilities of this set of analysis tools. This extension incorporates the following commands: (I) Choose SU, (II) GwObservationQuery and (III) Pumping and tracer Query.

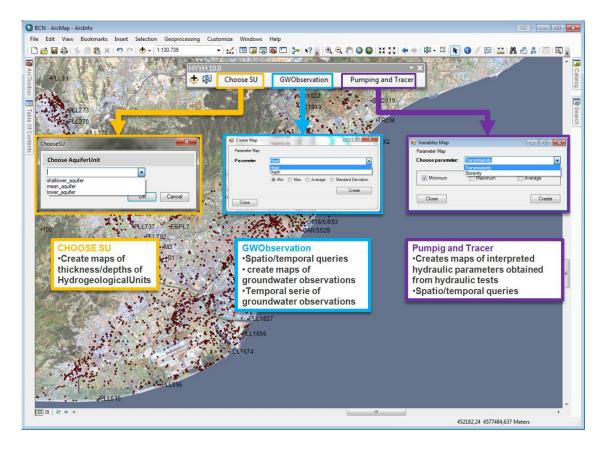


Figure 2.5. Sketch representing the toolbar implemented in ArcMap and its main components (ChooseSU, GwObservations and Pumping and Tracer Query) created to facilitate the analysis and interpretation of the hydrogeological data.

#### I. ChooseSU

This command enables the user to query the different depth or thickness of the different hydrogeological units (e.g. aquifer, aquitards) interpreted for the selected boreholes, and to represent these values in a map as point features. Results can be interpolated to raster by using different methodologies in the same ArcGIS environment (See Fig.2.6) or in other external platforms. The selection of the boreholes on the screen can be performed by using any of the available select commands (e.g. select by location or by rectangle) of ArcMap.

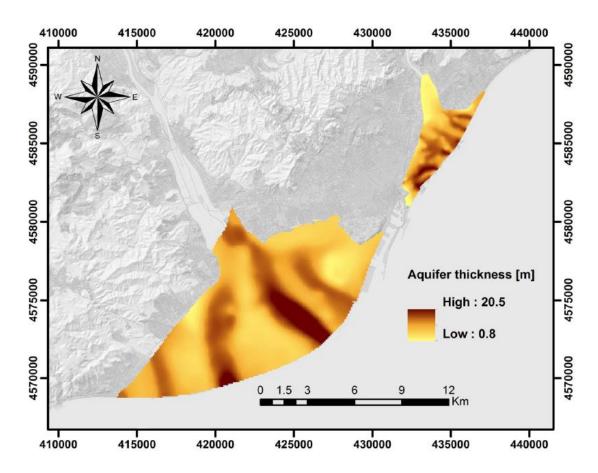


Figure 2.6. Map representing the main Aquifers thickness of the Besòs Delta Complex and of the Llobregat Delta Complex included in the metropolitanean area of Barcelona (NE, Spain).

#### II. GwObservationQuery

This set of tools (see Fig.2.7) enables us to calculate the minimum, maximum, average and standard deviation for each selected parameter (e.g. head level, depth to the water level) for a given period of time and for a point or a group of selected points. Besides, it allows us to represent these values in a map as spatial features (the number of **GwPoints** with information used is also displayed in the map). As with the results of the aforementioned command, these can be easily used for further analyses in the same ArcMap environment (e.g. using *Geostatistical Analysis Tools*), or in other external platforms. The most commonly used procedure consists in using the map of points with its corresponding head measurement values as a basis for creating piezometrics maps (e.g. in Fig.2.8). The selection of the hydrogeological data to be analysed is performed in two steps. The first step is to select a point or a set of points on the screen that represents the GwPoints. Thereafter, the user selects the period of time that he/she wishes in the query form. Moreover, a plot where the temporal evolution of the parameter can be observed for a given point or group of points can be generated with another command included in this tool set. Additionally, the user can also

obtain the aforementioned calculations for different periods of time for a given observation point.

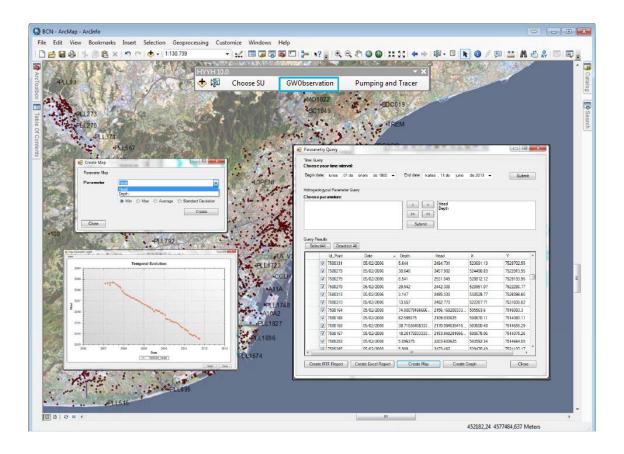


Figure 2.7. Sketch representing some utilities of the GwObservations command of HYYH.

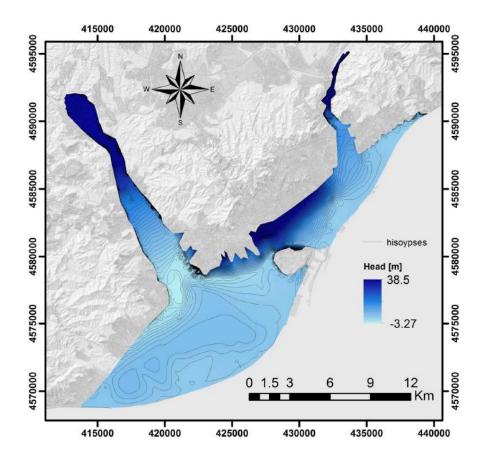


Figure 2.8. Piezometric map of the shallower aquifers of the urban area of Barcelona

#### III. Pumping and Tracer Query

This set of instruments was designed to facilitate the data retrieval of the groundwater points involved in a given pumping and/or tracer test (see Fig 2.9).

It consists on a multi-criteria query forms that enables the user to analize different data and interpretations derived from pumping and tracer tests (such as transmissivity, storativity, etc) and to represent these values in a map as point feature (see Fig.2.10). As results this maps can be analyze together with the values of permeability and transmissivity obtained by using the *Tools for the hydraulic conductivity estimation* (HEROS).

Finally, another utility of this module allows us to obtain the necessary information for the calculations performed with the EPHEBO/Maria J code. This code facilitates the pumping tests data interpretations by using a wide variety of methodologies. To date this procedure is still on-going.

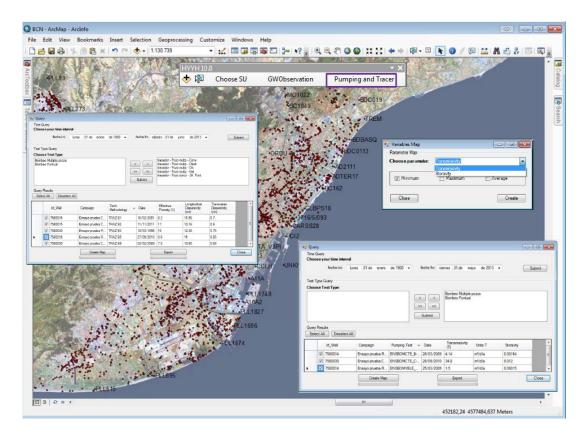


Figure 2.9. Sketch representing some utilities of the Pumping and Tracer tests Query command of HYYH.

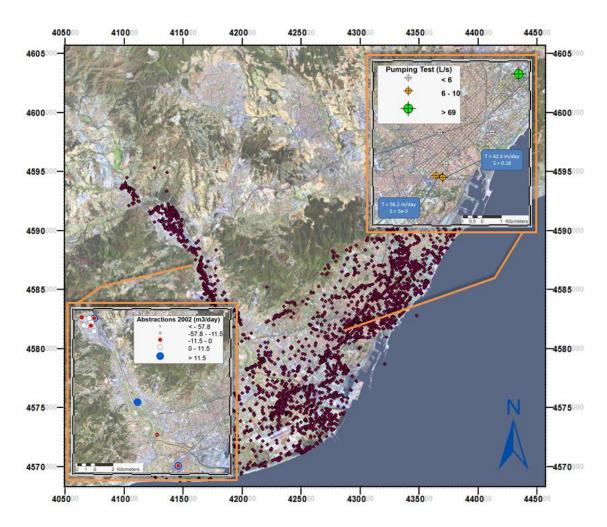


Figure 2.10. Map representing some values of abstractions and some results of hydraulic parameterization performed from pumping tests, queried and mapped by the HYYH tools in the urban area of Barcelona (NE Spain).

# 2.3.3 Storing the results: Interpreted data set.

This dataset represents the geometry and attributes of the different interpretations derived from the data stored in the database by using the aforementioned GIS-based tools and other inherent instruments provided by ArcGIS. This dataset is stored separately to allow additional interpretations and at the same time to act as a framework for a new project. In general terms, all the components include the following information: a) methodology used, b) the person/entity or poject responsible for the interpretation, c) date of the phenomenon and d) date when a version of the spatial objects was inserted or changed.

The feature classes and the rasters defined here can be exported to external platforms for further analyses. For instance, the hydrogeological units and their attributes can be exported directly (e.g. shapefiles) to Hydrogeological modeling platforms (e.g. Visual Transin).

Some efforts were made to import calculated meshes from some hydrogeological modelling platforms such as Visual Transin. This procedure is currently on-going.

This dataset is organised in 4 main datasets: I) GeoInterpretation, II) HydroInterpretations, III) GeoRasterDataset and IV) HydroRasterDataset.

#### I. GeoInterpretetations

This dataset was designed to store and structure the interpreted geological data, especially those obtained by using the *Geological Analysis Tools (HEROS)*. Consequently, the different geological elements (3D/2D lines, polygons and points) defined in each cross-section performed is stored in different tables whose attributes can be filled-up directly in this environment (see Fig.2.11).

#### I.1. GeolProfile

This line feature class includes the 2D spatial representation of the projection of the geological profiles generated by the *Stratigraphic cross-sections correlations tools (HEROS)* and other relevant information such as type of profile (e.g. projected, non-projected).

#### I.2. GeolUnitProfile3D/2D

The Stratigraphic cross-section correlation tools allow the user to export the geological units defined in the cross-sections as three dimensional polygons that can be stored in this feature-class. The attributes of this feature-class define the relative position of the units with respect to other units (top and bottom unit) and its main geological characteristics (e.g. geotechnical parameter). It is also possible to export and store the spatial representation of the geological units such as 2D polygons whose y-side represents the elevation and thickness of the unit.

### I.3. GeolStructureProfile3D/GeolStructureProfile2D

These line feature classes represent the geometries and attributes of the different structures such as faults, contact surfaces, etc defined in the geological profiles. In line with the GeolUnitProfile, these features can be exported as 3D elements or can maintain the 2D of the cross-section.

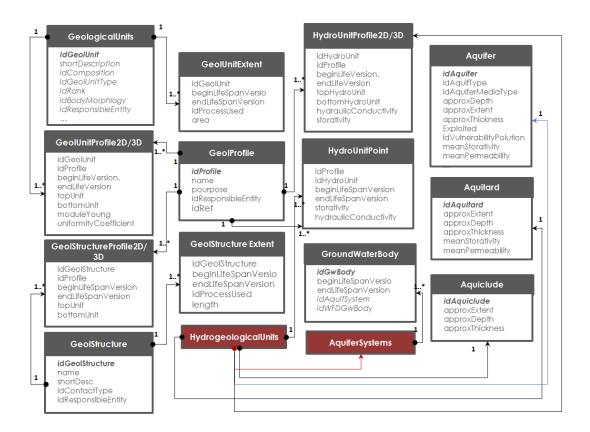


Figure 2.11. Simplified conceptual diagram representing some of principal contents of the interpreted dataset related to data obtained by using the *Stratigraphic cross-sections correlations tools* (HEROS).The 1 and 1..\* represents the cardinality of the relationships between tables.

#### I.4. GeolPointProfile3D

This 3D point feature class represents the spatial location of different punctual geological attributes observed in the cross-section and that are necessary for further analyses (e.g. location of a key sedimentary structure).

#### I.5. GeolUnitExtent and GeolStructureExtent

These feature classes represent the extension of the defined geological elements projected in the two dimensions of space. They were also designed to store previous geological elements defined by geological maps or other observations (e.g. aerial photographs).

Following the same scheme of the feature classes described above, the hydrogeological 2D and 3D elements defined in the cross-sections are stored in the tables HydroUnitProfile2D /3D feature-class. These feature classes represent the different 3D and 2D hydrogeological units (e.g. aquifers, aquitards, etc) identified in the cross-sections. The

attributes of these feature classes define the relative position of the units with respect to other units (top and bottom units) and their main hydrogeological characteristics (e.g. storativity, permeability). As with the geological units, the 3D hydrogeological units defined can be exported to hydrogeological modelling platforms for 3D modelling. In addition, the 2D polygons can also be exported together with their attributes to model specific archisymetric groundwater models.

#### II. <u>HydroInterpretations</u>

This dataset was designed to contain the derived interpretations and visualisations obtained by querying the database using the *Hydrogeological Analysis Tools (HYYH)*.

For instance, the features created using the command *GwObservation Query* (stored in **HydrogeologicalSurfacePoints**) contains the minimum, maximum, standard deviation and mean of the head level measurements for a given date and for a given groundwater points or group of points. If piezometric surfaces are interpreted from this information, they should be stored in **HydrogeologicalSurfaceLines** (see Fig.2.12).

Besides, the use of *Spatial Quimet Tools* (QUIMET) may provide the information necessary to produce the following maps required for the characterization of Groundwater bodies (WFD, 2009):

- Achievement/exceedence of good quantitative status
- Achievement/exceedence of good chemical status of Nitrates and of Pesticide.
- Achievement/exceedence of good chemical status based on national thresholds for other pollutants.
- Identification of GroundWaterBodies, where a significant and sustainable upward trend has been identified.

#### III. <u>GeoRasterDataset</u>

This raster dataset is commonly used to describe the top and the bottom boundary surfaces of the defined geological units and the spatial distribution of their geological distribution of properties. Rasters are usually created by interpolation of point observations. For the design of the structure of the Raster Catalog, the data model proposed by Strassberg, 2005 was taken into account.

# IV. <u>HydroRasterDataset</u>

This raster dataset is used to describe the top and the bottom boundary surfaces of the defined hydrogeological units and the spatial distribution of the hydrogeological properties (e.g. permeability, transmissivity). These properties can be obtained by using the *Tools that* 

calculate hydraulic parameters (HEROS) and/or the command of *Pumping and tracer Query* (HYYH).

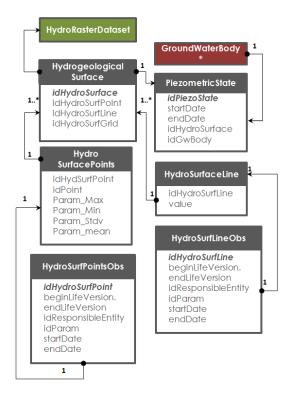


Figure 2.12. Simplified conceptual diagram representing some of principal contents of the interpreted dataset related to data obtained by using the commands of HYYH. The 1 and 1..\* represents the cardinality of the relationships between tables.

# 2.4 Application: urban area of Barcelona city (Spain)

The database model presented was implemented for the urban area of Barcelona. This spatial database together with the GIS-tools is designed to provide a regional framework for groundwater analysis in terms of both quantity and quality.

The urban area of Barcelona with a population over 5 million is located on the Mediterranean coast in the NE of the Iberian Peninsula (See Fig.2.12).

Geologically, the metropolitan area of Barcelona is formed basically by a coastal plain limited by two deltaic formations and a topographical higher area, the Catalan Coastal Ranges. The Catalan Coastal Ranges (which are mainly made up of Paleozoic rocks) in this area display a NE-SW direction and are limited by NE-SW and NW-SE normal and directional faults.

The Barcelona Costal Plain (Pujades et al., 2012) separates the two deltaic formations (Besòs Delta and Llobregat Delta), which consist of two Holocene depositional systems that were also active during the Pleistocene (Velasco et al., 2012b, Gamez et al., 2009). In general terms, these deltaic formations are constituted by several aquifers separated by lutitic units.

These aquifers have been used for irrigation and for industrial purposes in recent decades, posing a serious threat to the quantity and quality of the groundwater resources of the study area. Moreover, this region has an active underground infrastructure which compromised the quantity and quality of groundwater resources.

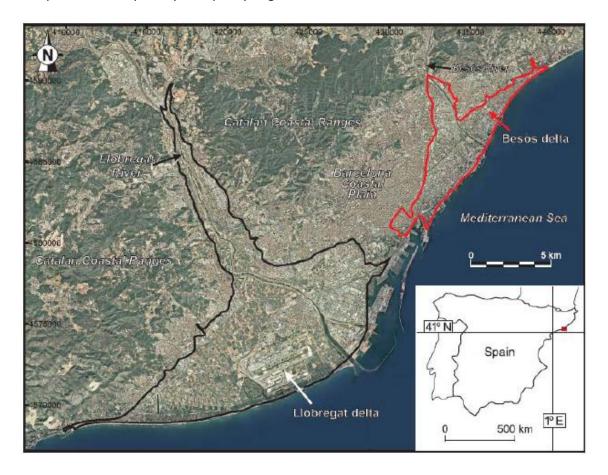


Figure 2.13. Orthophotograph of the metropolitan area of Barcelona covering the extent of the Besòs Delta, Llobregat Delta and Barcelona Coastal Plain.

# 2.4.1 Data recording

The information included in this database was collected mainly from the following sources:

• Existing geotechnical and hydrogeological reports (e.g. ADIF, 2007).

- National and regional Geological and Water Management Agencies such as Agencia Catalana d'I Aigua (ACA), Institut Cartogràfic de Catalunya (ICC), Institut Geològic de Catalunya (IGC), Instituto Geológico y Minero Español (IGME), Aigües Ter Llobregat (ATLL), Área Metropolitana de Barcelona (AMB) and Gestió d'Infraestructures, SA (GISA).
- Scientific experiments and modelling efforts performed by the Hydrogeological Group (GHS) of the Technical University of Catalonia (UPC) and CSIC (e.g. de Buen, 2009, Tubau et al., 2009).

All the data were analysed for transfer to a unified database taking into account the following aspects:

- Data format. Use of different data processing techniques for data from existing databases (spatial and non-spatial) or spreadsheets or paper format (e.g. geological maps, reports, etc).
- Data quality and reliability. Controls to prevent redundant and duplications were performed.
- Specific needs. Evaluation of specific analysis was performed to introduce new inputs into the database structure (e.g. data required for a geothermal study).
- Homogenisation and harmonisation of the data. For instance, in the geological description of the boreholes, it is common to find different description criteria that were unified by using intermediate tables and a proper entry protocol based on international standards.

#### 2.4.2 Dataset description

Within this work, the main geological data were obtained from 1442 boreholes owing to the scarcity of outcrops in the urban areas. Additionally, geophysical measurements such as gamma ray and other geotechnical measurements were also included in the database.

The principal hydrogeological data were obtained from wells and some mines. As a result, more than 3700 groundwater points were introduced (see figure 2.14). A range of approximately 90 years of time-dependent data was recorded including head level measurements and well abstractions. As for quality data, more than 5350 water samples obtained from different sources (e.g. groundwater points, rivers, and sewer) and their respective analyses were also recorded in the database.

Besides, a number of hydraulic test observations and their interpretations were also introduced into the database.

Other relevant information such as climatological information from 19 meteorological stations (see Fig.2.15) and further hydrological, geomorphological, geographical and administrative information were included in the database.

Finally, the database has at its disposal information provided by several hydrogeological and geological models performed in this area. This includes the regional geological model of the Besòs Delta (Velasco et al., 2012a) and more detailed geological and hydrogeological interpretations carried out at different studies sites in this zone (Velasco et al., 2012b; Riera et al., 2011; Escorcia, 2010). Moreover, other geological interpretations are provided for the Llobregat Delta (Gamez, 2007). Another study focused on the geothermal characterization of the urban area of Barcelona provides different geological and hydrogeological interpretations to the database (Garcia-Gil et al., 2013).

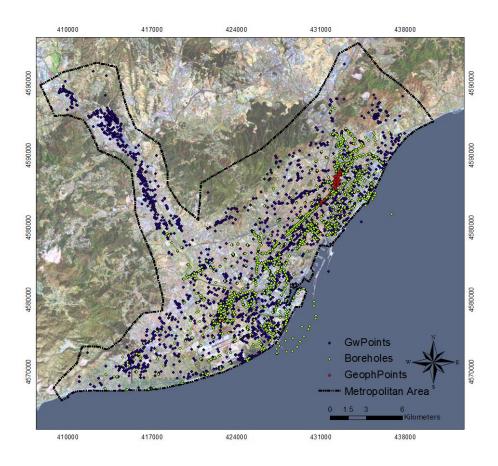


Figure 2.14. Map representing the spatial location of the groundwater points (GwPoints), of the boreholes (Boreholes) and of the Geophysical Points (GephPoints). In addition the metropolitan area of Barcelona is indicated by a dashed line.

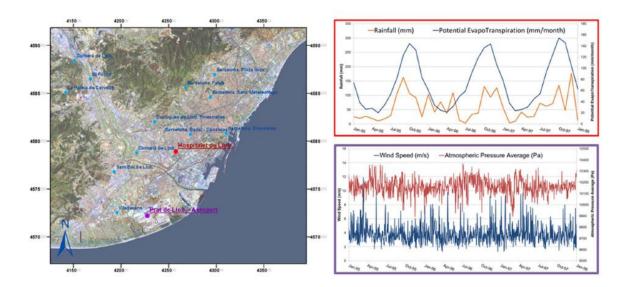


Figure 2.15.Map representing the location of the meteorological stations introduced in the HYDOR database in the urban area of Barcelona.

# 2.4.3 Data Query

The results provided in this section seeks to illustrate briefly how the database of Barcelona can be queried by using the GIS-tools, especially by using the Hydrogeological Analysis tools (HYYH). Further applications of the rest of the tools can be found in other works (Garcia-Gil et al., 2013; Velasco et al., 2013a; Velasco et al., 2012a; Velasco et al., 2012b; Riera et al., 2011; Escorcia, 2010)

First, 3D and 2D characterisations of the main aquifers of Barcelona were performed by using a combination of the *Geological Analysis Tools (HEROS)* and the *ChooseSU* command of HYYH. Thus, a 3D model of the different aquifers of the urban area of Barcelona is shown in Figure 2.16. A 2D representation of the main aquifers of the Llobregat and Besòs deltaic systems is also llustrateds in Figure 2.6.

Secondly, a piezometric map for this area was obtained with the help of the command *GwObservations Query* (HYYH) as shown in Fig 2.8.

Finally, the figure 2.10 illustrates some results provided by the application of the *Pumping and Tracer Query command* (HYYH) in the study area.

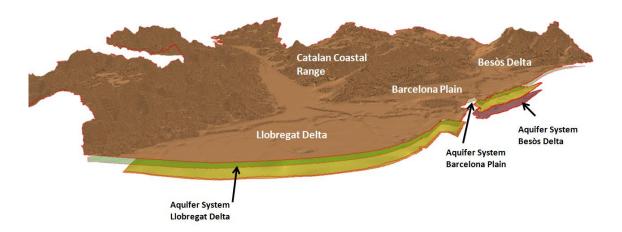


Figure 2.16. 3D model of the main aquifers layers in the urban area of Barcelona visualized in ArcScene (ArcGIS; ESRI). The interpretation and the 3D characterization were performed by using a combination of the Geological Analysis Tools (HEROS) and the ChooseSU command of HYYH.

#### 2.5 Conclusions and discussion

The GIS-based software platform presented in this chapter offers a user friendly environment with a large variety of automatic instruments designed specially for the management, analysis and interpretation of hydrogeological data.

The database (HYDOR) enables the integration and management of a wide variety of data focused on hydrogeological, hydrological, hydrometeorological, geological and other environmental information. However, some research is still warranted in the management of other data concerning groundwater characterization. For instance, as regards the geophysical component of the database, further types of geophysical data such as seismic reflection data together with the derived models are planned to be introduced into future versions of the database.

Although not all data types and structures are supported, the design of the database offers flexibility as it allows its extension and customisation to be used in further environmental and geoscientific applications. For example, further adjustments of the database to allow the storage of data from the  $CO_2$  injection sites are planned.

The introduction of data is facilitated by alternative utilities such as intermediate tables, inherent GIS wizards and assisting menus following a pre-established entry protocol.

As regards the implementation of the recommendations established by the European Community (e.g. INSPIRE) to ensure data exchange, some steps have been accomplished.

Despite the possibility of storing a large amount of data, the consultation of the data is simple when using the following GIS-tools that enable the visualization and analysis of

hydrogeological data. HEROS, allows us to perform a detailed geological analysis and the 3D representation of the interpreted geological features. QUIMET incorporates a wide range of instruments for hydrochemical analysis and HYYH comprises utilities for the analysis of hydrogeological and hydraulic experimental data.

These tools were implemented in the same ArcGIS software package and their analysis potential was extended taking advantage of the additional inbuilt instruments of this platform (e.g. Geostatistical tools, Spatial Analysis tools). Furthermore, ArcGIS fosters a shallow learning curve, the easy maintenance and the interoperability among different tools owing to its widespread adoption.

The interpreted data and calculations can be easily stored and consulted in the same platform and can be used to build an updatable model database for further interpretations. Thus, each new study does not have to start from scratch.

This software platform offers interoperability with external software for further analyses of the hydrogeological data, such as hydrochemical modelling packages like MIX code. Moreover, with certain adjustments this software platform could be easily linked to other programs such as PHREEQC, SGeMs, and TRANSIN considerably increasing the variety of hydrogeological calculations.

The application of the database model (HYDOR) for the urban environment of Barcelona provided an efficient framework for groundwater studies that can be updated and downscaled. 3D and 2D representations of the main aquifer boundaries of the study area were obtained by combining the aforementioned tools. Moreover, piezometric maps can be easily generated for the desired time intervals. Additional downscaling studies were performed in selected areas of Barcelona (e.g. detailed geological model of the Besòs Delta, hydrochemical analysis of the Badalona urban area).

# 3 THE USE OF GIS-BASED 3D GEOLOGICAL TOOLS TO IMPROVE HYDROGEOLOGICAL MODELS OF SEDIMENTARY MEDIA IN AN URBAN ENVIRONMENT

#### 3.1 Introduction

Sedimentary media (alluvial sediments, deltas, etc.) constitute important aquifers because of their high permeability, storage capacity, and interaction with surface water. In an urban environment, there is a considerable impact of human activity in terms of quality and quantity on groundwater (due to the sewerage system, the water supply network, etc.). Moreover, groundwater poses a problem for the development of infrastructure such as tunnels, basement crossings of large buildings, underground parking lots, etc (Vázquez- Suñè et al., 2005, Pujades et al., 2011).

Groundwater models constitute an essential tool for a reliable water management in urban sedimentary media (Pokrajac 1999; Vázquez-Suñé et al., 2006; Carneiro and Carvalho 2010). These models allow us to conceptualize, identify and quantify the hydrogeological processes. They enable us to simulate various scenarios such as droughts, water resource exploitation, water quality evolution and interaction with civil works in terms of hydraulic and geomechanical behaviour of the ground.

Hydrogeological modeling simulates the aforementioned processes provided that: (1) the geometry and connectivity of the different sedimentary bodies are known (thus the distribution of the hydraulic conductivity, porosity and other hydraulic relevant properties will be correctly characterized), (2) the petrophysics and hydraulic parameters of the sedimentary media are correctly estimated, and (3) the geometry and properties are adequately implemented into hydrogeological model.

The first two points focus mainly on the geological modeling as a first step in hydrogeological analysis. The last point highlights the need for reliable tools to implement the geological model and its properties into the hydrogeological model.

This chapter is based in Velasco, V., Gogu, R., Vázquez-Suñè, E., Garriga, a., Ramos, E., Riera, J., & Alcaraz, M. (2012). The use of GIS-based 3D geological tools to improve hydrogeological models of sedimentary media in an urban environment. Environmental Earth Sciences. doi:10.1007/s12665-012-1898-2

In the absence of a detailed stratigraphic interpretation, the geological modeling of the heterogeneous sedimentary media will be incomplete or will fail. A detailed stratigraphic analysis can be performed only if sufficient data are available.

Thus, the first step in geological modeling is to collect, sort and then select usable geological data (Kauffman and Martin 2008).

Traditional geological data such as two dimensional (2D) maps (geological maps, profiles and contour maps) are used to help geologists address practical problems. However, geological information essentially exists in three dimensions (Ming et al., 2010). The integration of original geological data and the reconstruction of their 3D shape in a 3D model will provide a reliable spatial representation of the geological variability, thus improving the hydrogeological models. This aspect has been emphasized by many authors such as Robin et al., 2005; Ross et al. 2005, Wycisk et al., 2009, and Velasco et al., 2012a.

In many subsurface modelling studies, especially those concerning urban areas, some specific issues focusing on the gathering and the management of usable geological data should be addressed:

- (1) Outcrops are often infrequent and available subsurface data come from different sources (building foundations, roads, underground infrastructures, research campaigns, etc) and are normally very heterogeneous (Rienzo et al., 2008) in both format (borehole logs, records of drilling parameters, etc.) and description (depending on the knowledge of the professional, the accuracy of the instruments, etc)
- (2) Despite the limited information because of continuing urbanization, there is usually a vast legacy of available geological information (Culshaw and Price, 2011) including previous geological interpretations and older raw data. Interpretations of geological observations depend not only on the observer and work scale but also on geological knowledge at the time of interpretation. Therefore, reinterpretation may be needed in order to use this information (Kauffmann and Martin 2008). To this end, a suitable system of data storage, management and validation is essential.

Once the geological model is constructed, further hydrogeological information constituted by a large amount of different data (chemical and heads measurements, hydrogeological tests results, etc.) must be integrated to complete the hydrogeological conceptual model.

This large pool of diverse subsurface data cannot be easily handled and analyzed without a unified database and software that allows interactive display and visual correlation. Geographic Information System (GIS) based software is one of the solutions for the management and analysis of geological and hydrogeological data since most of these data refer to locations on the Earth and such spatial complexity can be well accommodated in GIS (Chang and Park 2004, Wu et al., 2008, Chaaban et al., 2012).

[Chapter 3: The use of GIS-based 3D geological tools to improve hydrogeological models of sedimentary media in an urban aquifer.]

This paper presents a software platform that integrates a spatial database and a set of tools and methodologies developed in a GIS environment with the aim of facilitating the development of 3D geological models of sedimentary media for hydrogeological modeling, especially in urban environments.

This set of tools and methodologies allow the user to 1) edit and visualize 3D data, 2) use the inherent query and retrieval facilities offered by GIS software, and 3) employ the resulting geological model in support of the hydraulic parameterization for hydrogeological modeling.

These technologies were applied to some studies in urbanized areas such as Barcelona, Spain (for further information see Escorcia 2010, Riera 2011 and Velasco et al., 2012a) and Bucharest, Romania (for further information see Gogu et al., 2011). Here, a study case located in a part of the Besòs Delta in the metropolitan area of Barcelona (Spain) is discussed in order to illustrate an application of the presented tools and methodologies.

# 3.2 Software instruments and spatial database concepts for geological analysis

Commercial and research instruments that assist the creation of 3D geological models are found in different software packages. These tools may be classified on the basis of their background philosophy as Computer Aided Design (CAD) packages and Geographical Information System (GIS) software. Geological analysis tools have been developed inside both software families. As a result, there is a marked difference between different software packages in accordance with their origin. A reliable geological modeling software platform should include both GIS and CAD instruments. This should be based on the spatial data storage, query, and retrieval facilities offered by GIS software and on the abilities of 3D data editing and visualization provided by CAD. Both software families (CAD and GIS) are currently expanding their functionalities. Particular CAD abilities are implemented in GIS software and database management facilities are implemented in CAD based products. CAD software was not designed to handle spatial data structures needed to provide reliable and accurate geological description (which is one of the main advantages of using GIS instead CAD) and GIS packages are still deficient in complex data editing and 3D analysis and visualization. A short review of some of these packages underlines the need for the work to be performed. This begins by reviewing some professional stand-alone CAD based software packages, paying particular attention to GIS based software in the second part of this section. Software like Earthvision (Earthvision, 2012), Vulcan (Vulcan, 2012), 3D Geomodeller (3dGeomodeller, 2008), EVS and MVS (EVS and MVS, 2012) as well as other powerful packages can be added. Nevertheless, this review is not intended to be exhaustive.

 GOCAD (Gocad, 2011) is a large and complex geological modeling software package based on CAD technology. Its main module is focused on structural modeling, allowing

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geological cross-sections and map generation. The basic module offers an analysis platform for seismic data tests. Additional modules support specific tasks such as 2D or 3D grid construction and time-to-depth conversions by modeling the entire geologic column, or merging seismic interpretation with structural modeling, or constructing pillar based stratigraphic grids for geostatistic and flow simulation.

- Leapfrog software (Leapfrog3D, 2012) has been developed for 3D modeling of drill-hole data and for the construction of 3D geological models. Leapfrog generates wireframe models of lithology, alteration and mineralization, which can be exported to other mining software packages. Existing maps and cross-sections can also be viewed in its 3D environment. The Leapfrog 3D models can be exported to a variety of CAD software formats as for example dxf, Vulcan, or GOCAD. Additionally, Leapfrog 3D can import pre-selected structures from interpreted seismic images or any of the common GIS output formats.
- Rockworks (Rockworks, 2012) software offers a specialized modeling method that allows a lithology model interpolation. Its algorithms can be used to interpolate continuous stratigraphic surfaces, which when stacked, form a 3D stratigraphic model. Other functions enable the user to create individual logs or multi-logs cross sections, fence-diagrams and maps in 2D and 3D. Furthermore, it provides some GIS processing tools as well as import/export capabilities in various formats.
- HydroGeo Analyst (Hydrogeoanalyst, 2011), developed by Schlumberger Water Services, is designed for groundwater and environmental data management. It uses the SQL Server as its database and the construction of plots entails the use of one program to generate and execute a SQL statement and then a second program for data mapping. It enables us to display borehole logs, and permits the interpretation of cross sections. The software supports some steps of data pre-processing in modelling 3D groundwater flow and contaminant transport by defining hydrological layers interpreted from borehole logs. Its map manager allows us to exchange geographical information and uses GIS mapping technology.

Thus, any complicated 3D model can be constructed in principle using the aforementioned editing tools by employing CAD based package software. However, GIS based tools developed for geological analyses are especially suited for managing spatial data in terms of information query and retrieval. The need for querying tools emerged as a way of visually sorting and grouping the data to find areas that have certain characteristics and yield insights from their locations and distribution (McCarthy and Graniero 2006). This is systematically applied to working hypotheses regarding geological processes by outlining the relative values, frequencies, or distributions of some attributes across different lithologies or formations. In this regard, some of GIS based software packages for geological analysis are reviewed below.

#### 3.2.1 GIS based software packages for geological analysis

GIS based packages for geological analysis depend on the spatial database structure on which they are based. There are several concepts and developments of structuring geological spatial information for hydrogeological studies (Barazzuoli ,1999; Gogu et al., 2001; de Dreuzy et al., 2006; Carrera-Hernandez and Gaskin 2008; Comunian and Renar 2009; Wodjda et al., 2010, Chesnaux et al .,2011). However, there are few spatial data structures that allow a very detailed stratigraphic analysis and most of them do not have the necessary tools to exploit the information. Two examples of efforts in structuring stratigraphic data were considered significant and they are discussed in the following paragraphs:

- The Subcommission on Stratigraphic Information System forms part of the International Commission on Stratigraphy (ICS, 2012), which is an organisation concerned with stratigraphy on a global scale. This commission organizes the stratigraphic information in a number of ways: Geological and biological events and Earth history, Facies stratigraphy, Paleostratigraphic and Paleoclimatics maps (continental and marine ecosystems), and Iconographic Atlases (Index fossils species and Biostratigraphy in thin-sections). It also organizes the Geological Time Scale Information and Stratigraphic standards and Lexicons.
- The other example is the coal-related Stratigraphic database developed by the Coal Section of the Illinois State Geological Survey (Illinois State Geological Survey, 2012). The database is designed to store drill-hole log data and the description of outcrops and of mine exposures. Various stratigraphic characteristics are represented within the database: outcrop descriptions, cores, geophysical logs, driller logs, and mine exposures. Multiple descriptions of the same exposure or drill hole are possible.

Some commercial software packages discussed below are examples of tools developed to exploit the geological information in a GIS environment to construct geological models.

Target for ArcGIS 3.5 (Geosoft, 2011) was produced to allow visualization and analysis
of borehole log data within the GIS environment. It has several functionalities that
allow surface and borehole mapping that regroups a subsurface 3D viewer and tools to
carry out borehole plans, cross-sections, surface mapping and professional map
production.

While this system contains many powerful features for performing geological analysis, it has not been based in a comprehensive predefined geodatabase to facilitate the integration and representation of detailed stratigraphic data with hydrogeological data.

Part of the EquIS (Earthsoft, 2012) software platform produced by EarthSoft is EquIS
 3D Geology. The platform is fairly complex and allows us to view the lithology data in
 2D or 3D. The ArcGIS (ESRI) software module adds modules and utilities to enhance

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the capabilities of ArcMap and ArcScene applications. The GIS functionalities therefore create, query, map, analyze, and report from the EQuIS project databases. Visualization of borehole logs is done by querying the database on the GIS platform and using gINT (Gintsoftware, 2011) software.2D cross-sections are performed by using a RockWorks package or by creating a duty cross-section in gINT software package. In the ArcGIS (ESRI) module, Arc Scene, the users can visualize the output from RockWorks 3D fence diagrams, which EQuIS transfers to either shapefile or a personal geodatabase (ESRI) format. For advanced 3D visualization, EQuIS for ArcGIS is integrated with EVS software packages (CTech's 3D). Results from spatial queries and lithology information for boreholes are exported to EVS compatible format and thumbnails of various visualizing scenarios can be carried out. Because of the well defined integration within ArcGIS, it can use its geostatistic and spatial analysis modules.

 RockWare GIS link 2 (RockWare GIS link 2, 2012) imports the borehole location into ArcMap and enables us to generate cross-sections, fence-diagrams, logs, isopach and contour maps using ArcMap and Rockworks.

Although these software packages may be very useful for developing three-dimensional geological models, the use of third party software to perform a detailed stratigraphic analysis complicates the procedure and increase the cost of the product.

• The British Geological survey concept "Geological Surveying and Investigation in 3 dimensions" (GSI3D) involves a methodology and an associated software tool for 3D geological modeling (Kessler et al., 2009). The software is written in Java and data are stored in extensible mark-up language XML. GSI3D uses a digital elevation model, surface geological linework, and borehole data to enable the geologist to construct cross sections by correlating boreholes and outcrops. Mathematical interpolation between the nodes along the drawn sections and the limits of the units produces a solid model comprising a stack of triangulated objects, each corresponding to one of the geological units present. The user can construct cross sections automatically where it is possible to perform borehole correlations.

Other research tools have been developed in a similar vein. Some of them are discussed in the following paragraph.

McCarty and Graniero, 2006 developed a tool (BorelS) to aid in the management, visualization, querying and analysis of borehole data building in ESRI's established ArcScene software. Creation and visualization of cross-section for its further interpretation was not possible.

Whiteaker et al., 2012 recently develop a GIS data model and tools for creating and working with a 2D cross-section. The data model and tools create a framework that can be

applied using ESRI's ArcGIS software. Additionally, the 2D cross-sections are converted to 3D fence-diagrams and displayed in ArcScene. This system is complete and powerful since it integrates this set of tools with other features related to site characterization in the GIS (using ArcHydro Groundwater data model). However, it does not contain specific tools to develop a detailed sedimentary media stratigraphic analysis. For instance, the geological cross sections do not show some stratigraphic details that are useful in performing accurate the stratigraphic correlations.

# 3.3 GIS-based platform for 3D geological analysis

## 3.3.1 Design goals

The main difficulty for geologists has been to depict a three-dimensional system through a two-dimensional media, traditionally on paper, and in recent years with Geographical Information Systems (GIS).

The creation of two dimensional profiles constructed from well log data resolves the problem of showing 3D objects in 2D and constitutes an optimum framework for performing geological interpretations by borehole correlation.

The correlation of borehole data entails a combination of subjective and objective examinations of processes based on stratigraphic analysis, interpretations and assumptions that can lead to a geological model with some uncertainties (Borgomano et al. 2008).

Furthermore, the geological interpretation derived from 2D cross-sections can be transferred to 3D by aligning profiles along different cross-sections, thus creating a 3D view of the entire model.

It should be pointed out that the accuracy of the correlation depends on the quantity and the quality of the available well log data and on the geological interpretation.

To make the evaluation of the data more realistic, it is also important to be able to integrate and compare different types of data related to the geology of a site. For instance, when reading and interpreting geophysical logs it is possible to corroborate these data with other data from lithological boreholes or available samples.

Accordingly, an accurate stratigraphic interpretation of a site demands 1) the availability of sufficient data, 2) tools that facilitate homogenization, integration and query of these data, and 3) the availability of suitable tools and methodologies to interpret these data in a 3D environment.

In the light of the foregoing discussion, a software platform that brings together the tools and methodologies to facilitate an accurate stratigraphic analysis for the subsequent development of 3D geological model was developed. These tools, which were developed within a GIS environment, enable us to construct a geological model with several techniques and allow us to implement this information into flow and transport models. To this end, the following technical requirements should be fulfilled:

- I. Management and storage of spatial features and time-dependent data on a geospatial database.
- II. Stratigraphic interpretation and analysis of geological data by using:
  - II.1. Typical queries and visualization of data in a GIS environment.
  - II.2. Specific instruments to perform accurate stratigraphic analysis: Visualization of stratigraphic columns and generation of cross section.
  - II.3. Different geostatistics tools.
  - II.4. Typical capabilities of GIS for interaction with other features and creation of thematic maps.
- III. Creation of 3D geological models by using:
  - III.1. Different modeling approaches (deterministic or stochastic)
  - III.2. Tools to generate 3D surfaces of isopachs and isobaths maps in a GIS environment
  - III.3. Tools to generate fence-diagrams in a GIS environment
- IV. Hydraulic parameterization based on the petrophysical distribution of the geological units by using tools that enable us to:
  - IV.1. Calculate hydraulic properties from the stored data.
  - IV.2. Import/export hydraulic parameters.
- V. Facility of interaction with external software such as:
  - V.1. Geostatistic software such as SGEMS (Remy et al 2009) or GSLIB (Deutch and Journal, 1998)
  - V.2. Groundwater modeling packages such as TRANSIN (Medina and Carrera, 2003, Medina et al., 2000)
  - V.3. Pre-processor package to generate 3D finite element mesh such as GID (CIMNE, 2012).
- VI. Post-processing by using:
  - VI.1. Maps, diagrams or queries in a GIS environment.

#### 3.3.2 Analysis software platform.

The 3D analysis platform for groundwater modeling is composed of a hydrogeological geospatial database (HYDOR) and several sets of instruments that enable us to perform an accurate stratigraphic analysis. These instruments were developed as an extension to the ESRI's ArcMap environment, which is part of the ArcGIS version 10 software packages. They were created with ArcObjects, which is a developer kit for ArcGIS based on Component Object

Model (COM) and they were programmed in a Visual Basic of Visual Studio (Microsoft) environment.

The analysis software platform was developed according to the following guidelines (See work-flow diagram; fig. 3.1):

- I. Collection of geological data in a hydrogeological database. This database follows the geodatabase structure provided by the ArcGIS (ESRI) concept for representing geospatial information. It stores geological and groundwater information about the sedimentary media.
- II. Interpretation of geological data and construction of a 3D geological model by using a set of instruments that use the database spatial information termed Lithological and Stratigraphic analysis tools to perform stratigraphic analysis. Its main components, which will be described in this section, are the Borehole diagram instruments and the Stratigraphic cross-sections correlation tool. These tools together with the deterministic methods and the import/export procedures to the Geostatistic software are shown in the work-flow diagram as being part of the Interpretation module.
- III. Parameterization of the geological model. This is mainly performed by another set of instruments termed Tools for the hydraulic conductivity initial estimation, which enables us to estimate the hydraulic conductivity of each lithological interval defined in the borehole and of the user defined stratigraphic units. In Fig. 3.1 these tools are represented by the Hydrogeological parameterization module and its interactions with the hydrogeological geospatial database.
- IV. Exportation of all these data to an external modeling platform. The results of the aforementioned model can be exported to another external platform.

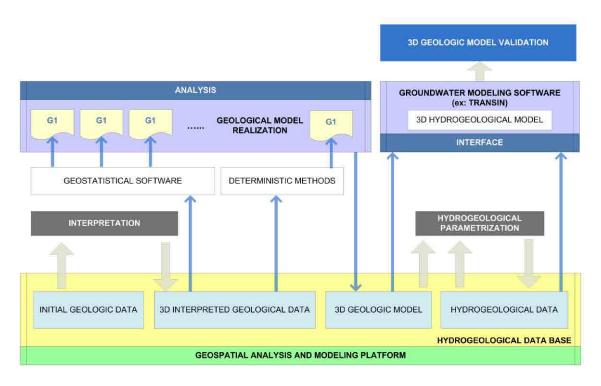


Figure 3.1. General scheme of the GIS based 3D geological analysis platform for groundwater modeling.

#### 3.3.2.1 Hydrogeological Geospatial Database

The geospatial database design has an Object-Oriented approach and is easily extensible. An important step in the development of the database process was the creation of a conceptual model of the required information. A wide range of data was identified: geography, geology, hydrology, hydrogeology, meteorology, water engineering, land management and others. Existing projects and data models were also explored in order to identify possible interactions and contributions.

The architecture of the hydrogeological database is in accordance with international standards concerning geospatial data encoding and transfer. This is reflected in its object-oriented approach supported by the Open Geospatial Consortium (OGC) and the International Organisation for Standardization (ISO).

Several existing patterns or data models were explored and are listed below:

- The Australian National Groundwater Data Transfer Standard, (1999).
- HYGES hydrogeological database of University of Liege (Gogu et al., 2001).
- ArcHydro: ESRI hydrological data model (Maidment, 2002).

- Water Framework Directive and its Geospatial information working group (Vogt, 2002).
- GML: Geography Markup Language (Lake ,2005).
- GeoSciML, a generic Geoscience Mark-up Language (Sen and Duffy 2005).
- Groundwater Model of University of Texas, (Strassberg, 2005).
- XMML (eXploration and Mining Markup Language) as a GML application schema (Cox, 2004; XMML, 2006).

Based on these models a new and more comprehensive was prepared. This model characterizes additional hydrogeological information that is better suited to the particularities of the sedimentary media.

The main components of the hydrogeological database include groundwater features, hydrographic, drainage and geologic features. The details of the hydrogeological database fall beyond the scope of this paper (see Velasco et al., 2013a and Velasco et al., 2013b). However, further details of the geological components of the database and its relations is here given in order to illustrate the presented modeling platform.

The database structure allows us to store an accurate and very detailed geological description that can be generalized and upscaled (Fig. 3.2).

Petrological characteristics are described for sediments in terms of textural (sediment size, sorting, roundness, matrix support), lithological type, colour, and others. Likewise, fossil contents, sedimentary structures and geological unit's chronology are also stored. Consequently, relationships between the petrological, paleontological and chronological data can be established. Moreover, geotechnical properties (N value from Standard Penetration Test, total core recovery, geotechnical samples) obtained from boreholes and electrical geophysical logs (gamma logs, spontaneous potential and resistivity logs) were also introduced into the database. Descriptions of boreholes or samples and their interpretations are stored separately, thus allowing further reinterpretations.

The general frame of the database scheme was designed taking into consideration the existing hydrogeological model of the Llobregat Delta (Vázquez-Suñé et al., 2006) and the Barcelona plain (Tubau et al., 2010) both located in Barcelona (Spain).

[Chapter 3: The use of GIS-based 3D geological tools to improve hydrogeological models of sedimentary media in an urban aquifer.]

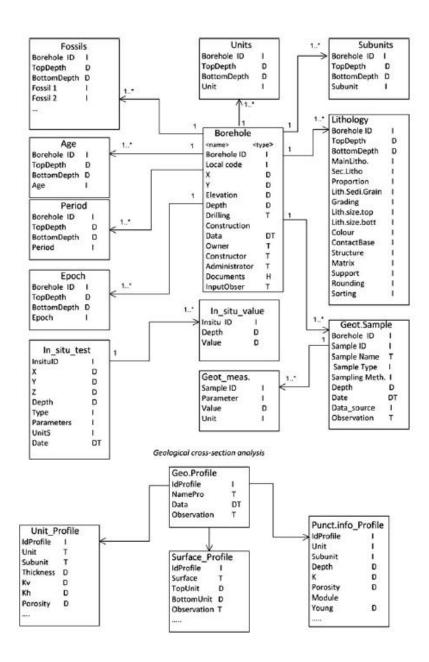


Figure 3.2. Simplified conceptual diagram representing the main geological contents of the hydrogeological geospatial database. The 1 and 1..\* represent the cardinality of the relationship between tables and I; Integer, D; double, DT; date, T; text.

# 3.3.2.2 Lithological and stratigraphic analysis tool

The instruments of lithological and stratigraphic analysis were designed to facilitate the interpretation of the geological data. As stated above, this set of tools consists of two subcomponents: 1) Borehole diagram instruments and 2) Stratigraphic cross-sections correlation tools.

Both extensions have the form of a toolbar tightly integrated within the ArcMap environment (ArcGIS, ESRI). (See fig. 3.3).

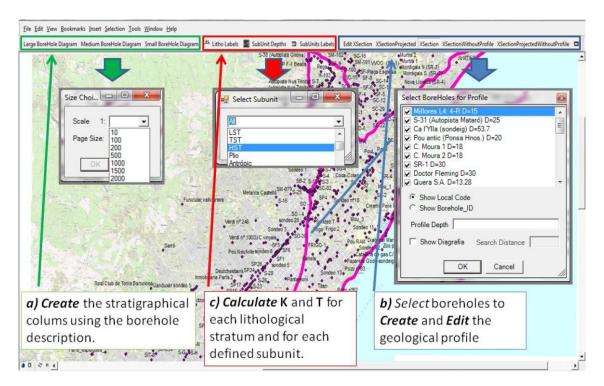


Figure 3.3. Sketch representing the toolbar implemented in ArcMap (ArcGIS, ESRI) of the three main sets of instruments created to facilitate the detailed stratigraphic analysis and the estimation of the sedimentary media hydraulic conductivity: a) Borehole diagram instruments; b) Stratigraphic cross-sections correlation tools; c) Tools for hydraulic conductivity initial estimation. For further details, please see epigraph 3.2.2.2 and 3.2.3.3 of section 3.3 (GIS based platform for 3D geological analysis)

# I. Borehole diagram instruments

This tool was developed to facilitate the visualization and the analysis of the detailed geological core description of the borehole. To make the analysis easier, data visualization was designed in line with the classic working environment of the geologist .By selecting a point that represents a borehole on the map, the user is able to query the attached lithological and stratigraphic information. In addition, the user can optionally attach information of geophysical in situ tests such as diagraphies. Fig. 3.4 shows, that for each lithological stratum, the petrological characteristics can be visualized in terms of texture (sediment size, sorting, roundness, and matrix support), lithology, and colour. The sedimentary structures, the geological layer boundaries, the subdivisions in units or subunits, their chronology and their paleontological content are also displayed.

The user can generate borehole core views in varying degrees of detail, at different vertical scales and in several paper formats. The resulting stratigraphic column diagram can

then be exported to various graphical formats. An example of a query resulting in a borehole diagram format is shown in fig. 3.5.

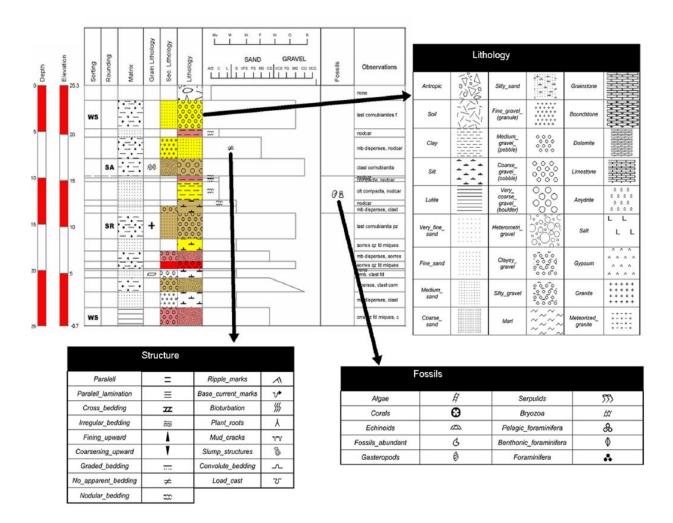


Figure 3.4. Scheme showing the representation of the petrological characteristics for sediments in terms of textural (sediment size, sorting, roundness, matrix support), lithological, colour, and other properties in a stratigraphic column obtained by using the tool Borehole Diagram.

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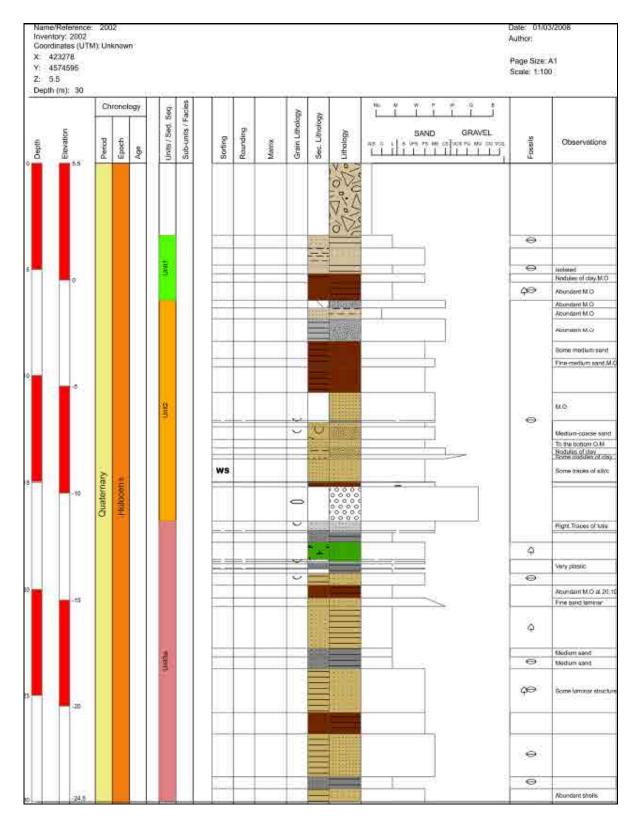


Figure 3.5. Result of the Borehole diagram query procedure. The lithology is defined by three components: Lithology (main lithology), secondary lithology and matrix. The proportion between the secondary and the main lithology is represented by the column labelled as Proportion, where W=with (same proportion of main and secondary lithology), F=frequent, S=some and T=traces

#### II. Stratigraphic cross-section correlation tool

This instrument facilitates the process of stratigraphic well correlation, in this way improving the geological interpretation of the sedimentary media.

It regroups a set of tools that starts from the creation of a geological profile (Fig.3.6) by querying a buffer zone line on a map that the user draws on the screen. A wizard opens and enables us to select certain cross-section properties such as buffer distance, labels of the boreholes (name or code), display of graphical results of in situ tests, vertical and horizontal scales, etc. The cross-sections can be created by keeping the distance between boreholes or by projecting them on a line. The profile is generated automatically by displaying the lithological columns of the boreholes together with the defined stratigraphic units/subunits and the graphical results of in situ tests. Complementary information such as the surface terrain profile extracted from the DEM, the distance between the boreholes, and the depth of each stratum is shown.

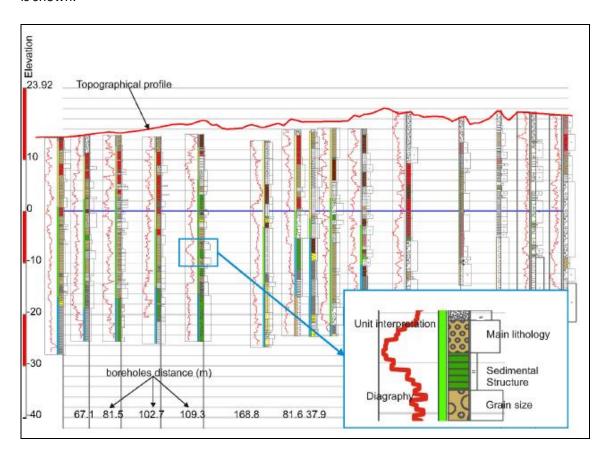


Figure 3.6. Geological profile generated by displaying the boreholes lithological columns together with the related stratigraphic subunits and diagraphies.

Thus, an interactive analysis environment (Fig.3.7) is created for a subsequent set of instruments. The user is able to analyze and to vectorize on screen the existing stratigraphic

elements by using lines, polygons, or points. It is possible to store a set of attributes such as the type of the contact, the position between the hydrogeological units or subunits, and different hydraulic parameters or other observations for each feature. Existing faults and fractures can be identified and drawn on screen within the same environment.

Although a cross-section is a 2D representation, the geological features defined by the user can be visualized in 3D in ArcScene. The export procedure provides spatial features such as points, lines, or polygons with their attached attributes. The visualization of several cross-sections describes a 3D panel forming part of a fence-diagram.

Using inherent editing tools of ArcGIS, the user can generate a raster surface representing the top and the bottom of the defined geological units.

The resulting 3D features can be exported to external software packages for further stochastic analysis or for constructing a geological 3D model.

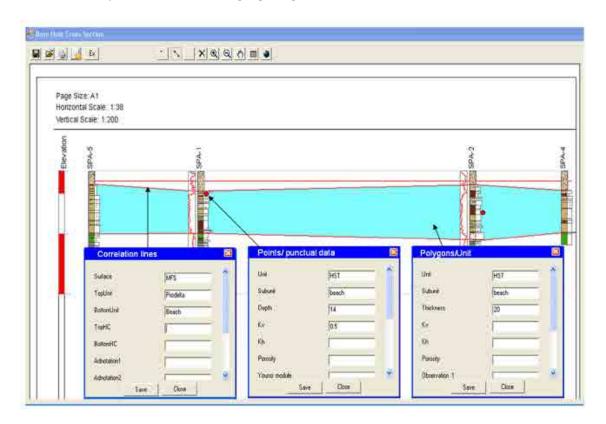


Figure 3.7. The stratigraphic working environment (the geologists draw their sections based on different borehole-log correlation techniques).

# 3.3.2.3 Tool for the hydraulic conductivity initial estimation

Hydraulic conductivity is a function of material texture although it specifically represents the ease of water flow through the porous media (Bonomi et al., 2009). Accordingly, several

steps were undertaken to quantify the hydraulic conductivity on the basis of grain size distribution.

Hydraulic conductivity can be computed automatically for each lithological interval defined in the boreholes or for the user defined hydrogeological units by using a set of tools. This was based on the existing lithological descriptions using different approach.

Each lithology listed in the database is associated with hydraulic conductivity values obtained from the literature (Freeze and Cherry 1979, Custodio and Llamas 1983). In the lithological table (Lithology; see fig. 3.2) the lithology of a downhole interval is defined by the main lithology field, the secondary lithology field and finally by the matrix field. Another field termed proportion provides the proportion of each lithology in this interval in terms of percentages.

An equivalent hydraulic conductivity can be calculated for each interval of the borehole, taking into account the permeability values assigned to each lithology and its grain size distribution in terms of percentages.

The approach adopted for the calculation of hydraulic conductivity of the defined units was based on the traditional calculation methods of hydrologically equivalent horizontal and vertical conductivity (Custodio and Llamas, 1983).

This methodology calculates the hydrologically equivalent horizontal hydraulic conductivity (kh) for the model units using:

$$(k_{\rm h}) = \frac{1}{L} \sum b_i \cdot k_i \tag{1}$$

where each lithological interval requires an assigned nominal hydraulic conductivity (ki) and the thickness of each interval (bi). Moreover, the unit thickness (L) is the sum of the thickness of each defined downhole interval:

$$L = \sum b_i \tag{2}$$

Furthermore the hydrologically equivalent vertical hydraulic conductivity (kv) for the model units is calculated by using:

$$1/k_v = \frac{1}{L} \sum_{i} \frac{b_i}{k_i}$$
 (3)

This approach has also been adopted by Brodie (1999).

Transmissivity values are also obtained automatically for each user defined unit/subunit by multiplying the unit thickness with its equivalent hydraulic permeability.

The values of hydraulic conductivity and transmissivity can be used as initial estimated values for the hydrogeological model or as an additional geostatistic analysis in the ArcGIS environment or in external software. The dating of this procedure is on-going.

# 3.4 Application

One application of the software platform is discussed in Velasco et al 20121. This consists in the geological and hydrogeological characterization of the entire emerged Besòs Delta (Barcelona, Spain) in addition to 5 Km from the coast line of the submerged part.

Owing to the location of the delta, part of which is occupied by the city of Barcelona, the region has undergone considerable urbanization. As a result, most of the previous existing rocky and sedimentary outcrops have disappeared. However, the recent increase in the number of geological, hydrogeological, and civil engineering works has provided a great deal of new data. Consequently, this constitutes an optimum moment for constructing a geological model that integrates a database storing several boreholes, in-situ tests, geotechnical, hydrogeological information and earlier geological interpretations, etc.

The Besòs delta is a depositional system created during the Quaternary by the sediments of the river Besòs. The deltaic succession shows an unconformity on a basement substratum formed by Palaeozoic and Cenozoic rocks, The Palaeozoic lithology consists mainly of slates and granite. The Cenozoic rocks are mostly made up of matrix-rich gravels and sandstones of Miocene age and of massive gray marls attributed to the Pliocene.

Like the neighbouring Llobregat river delta (Gámez et al. 2009), the Quaternary sedimentation of the Besòs river delta has been mainly controlled by sea-level changes, Quaternary glaciations and fault activity.

The geological model of the Besòs delta in this study is based on a sequence stratigraphic subdivision. This subdivision resulted from the identification of key stratigraphic surfaces and the general trends (progradational-retrogradational or coarsening-fining upwards) observed in the marine and transitional sediments in the boreholes.

In this work, we focus on a case study of a portion of the aforementioned geological model. We undertook a hydrogeological characterization of this area to evaluate the potential impact of an exploitation of the aquifers with the main aim of providing an alternative to the heating and refrigeration system at a building located in the study area (Barcelona, Spain).

The details of the hydrogeological model fall beyond the scope of this chapter. Only the creation of the geological model using the instruments and methodologies described is presented.

The location of the study area is shown in fig. 3.8a. Nine stratigraphic units forming part of the hydrogeology of the regional domain were identified (A to F2, Table 3.1).

First, the Borehole diagram instruments of the developed software platform enabled us to visualize and analyze the borehole log data and the geophysical log data in order to identify the aforementioned geological units.

The Stratigraphic cross-section correlation tools allowed us to correlate these units between the boreholes in six cross—sections. Fig. 3.8 a displays the borehole location, and the section lines and fig. 3.9 shows some of the resulting cross section.

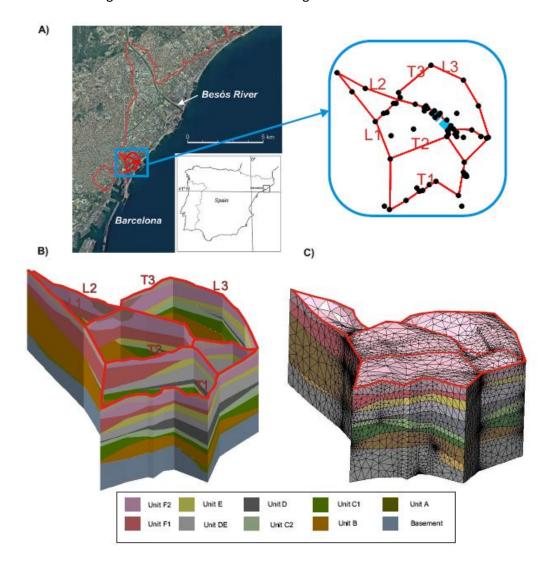


Figure 3.8. A) Location of the study area. The red line marks the boundary of the upper delta plain of the Besós river delta (Northeast Spain). The satellite image is provided by the Cartographical Institute of Catalonia. B) Geological model of the Besòs delta viewed by means of seven cross-sections generated, showing the geometry and continuity of the seven geological units distinguished. This model has been visualized in ArcScene. C) 3D geological model created by importing the 3D features defined with the developed instruments into the software platform GID.

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Age	Geological units	Sedimentary environmental deposits/facies association	Description
Post- glacial	F1	Delta plain (floodplain deposits)	Red and yellow clays
	F2	Delta plain (fluvial channel fill deposits and alluvial deposits)	Poorly sorted gravels, occasionally with sandy matrix and some lenses of organic matter. The pebbles are well rounded and polymictic
	Е	Regressive delta front	Yellow to grey coarse grained facies belt made up by sands and gravels (from distal to proximal). Shells fragments
	DE	Transition between prodelta and regressive delta front	Yellow to grey coarse sand with clayey/silty matrix. Shells fragments
	D	Prodelta	Grey clay and silts with intercalation of fine sand and with marine fauna
	C2	Transgressive delta front	Gravels well rounded to angular pebbles with sand. Shell fragments
	C1	Fluvial channel fill deposits (delta plain)	Poorly sorted gravels, occasionally with sandy matrix and some lenses of organic matter. The pebbles are well rounded and polymictic
Pleistocene	В	Delta plain (floodplain deposits and channel fill deposits)	Red and yellow clays intercalated with fluvial channel fill deposits which consist of poorly sorted gravels and sand with some lenses of organic matter
	A	Fluvial channel deposits	Poorly sorted gravels, occasionally with sandy to silty matrix. The pebbles are well rounded and polymictic

Table 3.1. Description of the facies association of the different geological units identify in the Besòs delta and in the model of the study area. Modify after Velasco et al 2012a.

On the basis of the features defined in the cross section, several raster layers and triangular network (TIN) corresponding to the top surface of each geological layer were created by using editing tools of ArcGIS.

With another set of editing tools of ArcGIS, isopachs maps were obtained from these raster layers and TIN. These surfaces with their attributes were then converted to shapefile and were directly exported to the groundwater modeling package Visual Transin which is a friendly user interface of TRANSIN to build up a quasi-3D hydrogeological model.

The next step was the hydraulic parameterization of the interpreted geological units. The definition of different zones of hydraulic conductivity were calculated taking into account and comparing the estimated values obtained with the hydraulic conductivity tools and the punctual values derived from hydraulic tests (performed in this study and earlier studies) stored in the hydrogeological database. Further insight into the study area can be obtained by visualizing subsurface features in a 3D environment. Fig.8 b shows the fence diagram in ArcScene obtained by visualizing the features defined in the cross-sections. The model developed by using the described GIS analysis instruments can also be used to construct a complete 3D geological model. Moreover, it can be exported to a numerical pre-processor to create a 3D hydrogeological model. To this end , GID software (CIMNE, 2012) developed by CIMNE Centre (Technical University of Barcelona) was selected as pre-processor to generate the 3D finite element mesh needed for groundwater modeling ( see figure 3.8 c).

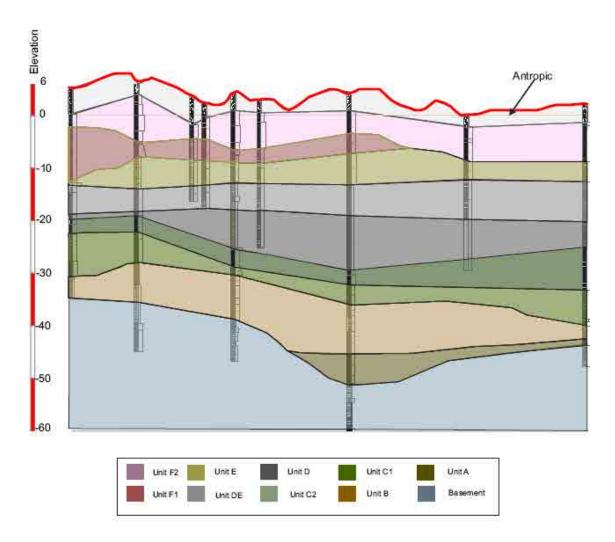


Figure 3.9. Cross-section parallel to the coast (T1, see figure 8a for location). The defined units can be visualized. See table 3.1, section 3.4 (Application) and for detailed description of the units.

# 3.5 Discussion and conclusion

This study presents a software platform representing a working environment to integrate 3D geological models of the sedimentary media in regular hydrogeological modeling methodologies. In line with this approach, several advantages should be highlighted. First, the structure of the spatial database allows us to store data for most geological and hydrogeological studies. This type of database has been designed to manipulate spatial and time-dependent information more efficiently than other platforms and allows the user to store and manage an accurate geological description that can be further upscaled.

In addition, the possibility of querying and visualizing the stored information allows the user to integrate all the data and thus obtain further relevant information. The integration of

detailed core stratigraphic and lithological descriptions with hydrogeological local and regional parameters, hydrogeological tests (pumping and tracer tests), hydrologic features and geophysical and geotechnical information, etc provides the user with a consistent image of the aquifer behaviour under study.

Another important advantage is that the use of the spatial database facilitates data integration concerning land-use, infrastructure design, and environmental aspects. The relationship between the groundwater and the main urban contaminant factors (sewerage system, water supply network, etc) and the interaction of the groundwater with major civil works (subway tunnels, underground parking lots, etc.) is highlighted. As a result, it is possible to study different problems in a more realistic manner in order to improve our understanding of the geology and hydrogeology of urban areas.

Apart from the database, the software platform contains several specific tools developed in ArcGIS (ESRI) designed to exploit the stored data. The use of these tools in combination with the ArcGIS capabilities increases the functionality of the software, which provides a comprehensive stratigraphic analysis and a subsequent geological modelization with a minimized learning curve.

One of these tools enables us to obtain stratigraphic columns, where relevant information such as texture, lithology, fossil content, chronology, results of in-situ test and earlier interpretations is shown together. This is an optimum environment for facilitating the interpretation and the identification of different sedimentary units / subunits.

The software platform also contains tools that support a variety of workflows for creating cross-sections. This system allows the modeling of the distribution and geometry of the sedimentary bodies by knowledge-based control of the modeler.

As shown in this paper, the 2D features defined in the cross sections can be converted into a 3D environment. The resulting 3D features can be visualized as fence-diagrams in the same GIS environment by using ArcScene or can be exported to external software packages to construct 3D geological models.

Despite these advances, there are still limitations in trying to construct 3D bodies using the 3D features defined in the cross-sections. This is especially true for sedimentary bodies, the geometry of which is very complex and/ or whose extent does not cover the whole area of the model (e.g., paleochannels).

Apart from these technical issues, the reliability of the geological model depends on the amount of data available, its nature and on its distribution over the area of interest.

This study seeks to provide a methodological approach and a set of tools for the detailed reconstruction of the hydraulic characteristics of sedimentary bodies.

Despite the fact that the hydraulic properties of the aquifers may be calculated automatically by using a set of tools, further work on these techniques should be conducted in this line in order to improve the usefulness of the platform presented.

Several features are planned for a future version of the software, which will extend its functionality.

This software platform enables us to set up an updatable model database for further downscaling. We used the Besòs Delta Model as a framework for the modelization of the study area. Likewise, some details extracted from the study area contributed to our understanding of the regional model.

The design of the tools presented is in line with the classic working instruments used by the geologist to characterize a study area. Although the main goal of the instruments described was to yield further insights into groundwater modeling of sedimentary media, the field of applications can be easily extended.

# 4 GIS-BASED HYDROGEOCHEMICAL ANALYSIS TOOLS (QUIMET)

# 4.1 Introduction

Water availability and accessibility must have an emphasis in qualitative aspects such as drinking water standards and required quality for different uses (Barthel et al 2008). In a given site the quality of groundwater may be adversely affected by factors such as industrialization, irrigation practices, or urbanization (Foster., 2001; Vazquez-Suñè et al., 2005b; Scanlon et al., 2005; Ketata et al., 2011). An accurate assessment of the negative impacts of these different activities is paramount for the protection of water bodies and ecosystems associated (Navarro-Ortega et al., 2012). In order to ensure compliance with standard regulatory guidelines (e.g., the European Water Frame Directive, WHO guidelines), continuous monitoring, evaluation, and interpretation of a large number of physical and chemical parameters is required. This involves: (a) determining the origin of groundwater and the processes controlling its chemical composition and the corresponding spatio-temporal distribution; (b) evaluating the current groundwater quality trend with reference to soil usage, soil type and hydrogeological setup; and (c) establishing the regional background composition of groundwater (in Mendizabal and Stuyfzand, 2009).

Accomplishing these tasks is not straightforward. The major difficulties faced in this area arise from: (i) the need to manipulate large data sets collected over many years; (ii) the integration of data stemming from diverse sources and gathered with different data access techniques and formats; iii) the management of data with varying quality standards and temporal and spatial extent; iv) data-handling derived from analysis and modeling, and v) the integration of groundwater quality information with other relevant information such as geological and other hydrogeological data.

Optimal data management of this vast amount of spatio-temporal information cannot be readily handled without the combination of a comprehensive geospatial database and a number of efficient technologies and methodologies capable of classifying, comparing, summarizing and interpreting huge data sets. Classic groundwater analysis techniques, including simple inspection and comparison of chemical analysis, spatio-temporal representation of the data, and preparation of hydrogeochemical diagrams, combined with statistical uni- and multivariate analysis, are convenient instruments for this purpose (Güler et al., 2002, Dreher, 2003).

This chapter is based in Velasco V, Tubau I, Vázquez-Suñè E, Gogu, R, Gaitanaru, D, Alcaraz, M, Serrano-Juan A, Fernàndez-Garcia D, Garrido T, Fraile J, Sanchez-Vila, X. GIS-based hydrogeochemical analysis tools (QUIMET). Submitted and accepted with revisions to Computers & Geosciences.

However, the choice of these methodologies cannot be easily predetermined a priori since this depends on the use, type and quality of the original data (Zaporozec, 1972, Morio et al., 2010). Moreover, the complexity and diversity of origins and processes associated with the large amount of chemical species monitored complicates the analysis of groundwater quality. Thus, we contend that a combination of the aforementioned methods plus an analysis that accounts for important auxiliary information (geology, hydrology, climate) and/or technologies (deeper geochemical analysis, modeling, geostatistical analysis) must be required in any complete hydrogeochemical analysis.

It comes as no surprise then that nowadays a great deal of software exist that can store, manipulate, and facilitate calculations and graphical data presentations in hydrogeochemical studies. Without being exhaustive, we can cite STATISTICA (Statsoft, 2013), SSPS (IBM, 2013), Minitab (Minitab, 2013), Stata (StataCorpLP, 2013), SAS/STAT software (SAS, 2012), Systat (Systac, 2008) or Microsoft Excel and MS Excel add-ins like BiPlot 1.1 (Udina, 2005). All of them provide a large variety of tools for correlation analysis, trend analysis and some also include multivariate statistical analysis to classify water samples.

Specialized hydrogeochemical analysis tools incorporating methodologies to process and interpret hydrogeochemical data such as the automatic creation of traditional diagrams and other specific calculations (ionic balance, ionic relations) are also available. These include free software codes like EASYQUIM (GHS, 2013), GW-Chart (USGS, 2013), or INAQUAS (ICOG, 2011). The last one also facilitates the classification of chemical species according to regulatory guidelines. Other software like AqQA (Rockware, 2013) generates conventional graphical plots related to chemical analyses and performs further calculations such as instant unit conversion, comparison of samples to laboratory standards and classification of the samples measurements according to regulatory limits. Similarly, Logicels (LHA, 2013) is a free software that also performs hydrogeochemical diagrams, ionic balance, and statistical analysis, but includes additional features such as isotopic calculations and neutralization simulation, and it is linked to the hydrogeochemical modeling software PHREEQC (Parkhurst and Appelo, 2013).

One advanced type of software is the commercial HyCA (KWR, 2011). This software incorporates a database as well as a map manager that allows the visualization of spatial data. HyCA can provide standard options such as time series, traditional hydrogeochemical diagrams and the creation of maps in planar view, cross sections and 3D information for any parameter in the database. Another example of advanced software is the commercial AQUACHEM (Schlumberger, 2013) .This platform has a fully customizable database of physical and chemical parameters and a comprehensive selection of analysis, calculation and modeling tools. In addition, it generates more than 20 standard graphical plots. Moreover, its map manager allows the complete visualization of data and results from their elaboration as well as geological and hydrogeological maps, etc. With respect to hydrogeochemical modeling, AQUACHEM has powerful geochemical reaction modeling capabilities by being coupled to PHREEQC.

The need for an effective management and retrieval of spatio-temporal dependent data has triggered the development of Geographical Information Systems (GIS) applications to hydrogeology (Goodchild et al., 1996, Martin et al., 2005). The use of GIS improves the visualization and edition of data through the simultaneous display of different layers or even more advanced 3D views. These types of applications improve the integration of quantitative and qualitative data and allow straightforward consultation, search, and retrieval of portions of information provided by different sources of spatial data (Descamps et al 2005).

Owing to advances in destock capabilities, programming languages and data availability, a number of GIS-based applications have been developed since the turn of the century for water analysis (e.g. Maidment, 2002; McKinney and Cai, 2002; Shen et al., 2005; Jia et al., 2009; Soutter et al., 2009; Strager et al., 2010; España et al., 2011), some of them emphasizing groundwater aspects (e.g.Gogu et al., 2001; Gemitzi and Tolikas, 2006; Steward and Bernard, 2006). In two most recent applications, Morio et al., 2010 introduced a GIS-based method to represent contaminant concentration distribution in groundwater based on different interpolation methods, and Rahman et al., 2012 developed a new spatial multi-criteria decision analysis software tool for selecting suitable sites for Managed Aquifer Recharge systems in a GIS environment. Another example of GIS-based tools is ArcHydro Groundwater tools (Aquaveo, 2012), which is based on the ArcHydro Groundwater data model (Strassberg, 2005) and takes advantage of the ArcGIS (ESRI, 2013) platform for archiving, managing and visualizing groundwater information. As regards groundwater quality analysis, ArcHydro enables the generation of water quality maps that can be linked to other hydrogeological information and to other thematic maps.

The aforementioned applications and software constitute important advances in the chemical analysis of groundwater. Nevertheless, the following issues remain to be resolved: (1) there is still a potential for improvement in tool development for hydrochemical analysis that combine graphical diagrams, specific queries and calculations; (2) methods necessary for a complete hydrogeochemical analysis have not yet been fully incorporated into a GIS environment in terms of in-built utilities for advanced temporal-spatial analyses; (3) there are a few geospatial databases designed especially for hydrogeochemical data management with the appropriate tools directly developed within a GIS environment.

To bridge these gaps, the main objective of this work is to present the QUIMET software platform, which integrates different tools that collect, analyze, treat, calculate and post-process hydrogeochemical data in a GIS environment with the tools for advanced temporal-spatial analyses directly built-in. The present study forms part of a wider on-going framework developed to facilitate detailed hydrogeological modeling studies of sedimentary media with hydrogeological and geological GIS—based analysis tools (Velasco et al., 2012b). The organization of the paper is as follows: First, section 4.2 presents the design and the software platform functionalities. Section 4.3 describes an application of this platform to a study area located in north-eastern Spain. The main conclusions arising from the application of the software together with its advantages and disadvantages are presented in Section 4.4.

# 4.2 GIS-based software platform QUIMET

# 4.2.1 Design approach

An effective methodology to interpret hydrogeochemical data should meet the following technical requirements:

- I. A geospatial database with appropriate data storage and management. The database structure should enable the storage and management of large hydrogeological time dependent data geographically referenced. Moreover, its structure should facilitate standardization and harmonization of raw data. This environment should include specific mechanisms for facilitating data transcription (i.e., "one by one", "massive"), managing different data formats, editing (such as duplicate removals), and the management of measurements reported in different units.
- II. Data processing and analysis. In order to perform an effective processing of the hydrogeochemical related data stored in the aforementioned database, the following instruments and/or methodologies should be available:
  - II.1. GIS environment for exploiting a vast range of capabilities including: (1) creation of spatio-temporal queries and calculations; (2) integration of different types of data settings (e.g. geological , hydrogeological data); (3) creation of interactive mapping; and (4) effective assessment of the legitimacy, consistency and correlation of the input data.
  - II.2. Instruments that facilitate the hydrogeochemical analysis by using quality control computation methods (e.g., ionic balance) and traditional graphical analysis techniques (e.g., Piper Diagram).
  - II.3. General statistical tools to process and validate data in order to generate different hypotheses for interpretation and presentation of the information in a compact format.
  - II.4. Different interpolation tools to estimate/validate the spatial distribution of the chemical/physical components.
- III. Native interaction with external software for further analysis of the hydrochemical data, such as Geochemical modeling packages like PHREEQC, NETPATH (Plummer et al., 1994), MIX (Carrera et al., 2004), Geostatistical codes/software such as SGeMs (Remy et al., 2009) or GsLIB (Deustch and Journel, 1998), and Groundwater modeling packages (either commercial or based on free software).
- IV. Post-processing tools: The results obtained from analyzing the hydrogeochemical data in an external platform (e.g., a given hydrogeochemical modeling platform), should

be easily imported again into the GIS environment for further analysis and data integration.

# 4.2.2 The Software platform QUIMET

The requirements enumerated in the previous section were adopted as guidelines during the design of the software platform devoted to the interpretation of hydrogeochemical data (QUIMET). QUIMET is composed of a geospatial database termed HYDOR (described in section 4.2.2.1 and in Velasco et al 2013b) plus a set of tools specifically designed for graphical and statistical analysis of hydrogeochemical parameters. This set of analysis tools is grouped into two main families: Spatial QUIMET (described in section 4.2.2.2) and Statistical QUIMET (described in section 4.2.2.3).

All these functionalities are integrated into a friendly graphical user interface (GUI). QUIMET, programmed in Visual Basic Programming Language (VBPL), is able to coordinate its activities with several external widespread software (ArcGIS, Microsoft Excel, and Microsoft Access). A sketch of the graphical interface is shown in Figure 4.1.

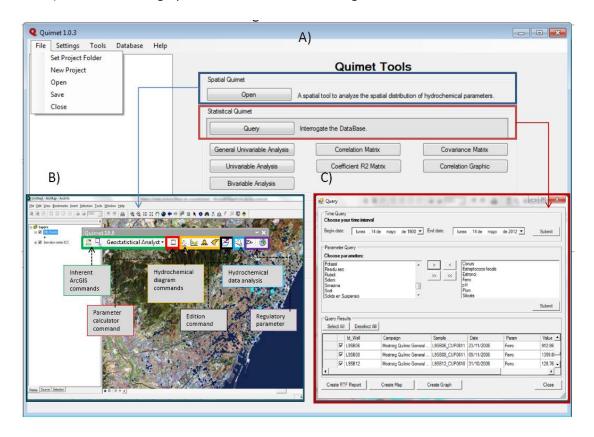


Figure 4.1. A) Graphical User's Interface (GUI) of QUIMET software platform. It coordinates its activities with several external software (ArcGIS, MS Excel, MS Access) and is composed of two main modules: Spatial Quimet and Statistical Quimet. B) Sketch representing the toolbar implemented in ArcMap (Spatial QUIMET module) and its main commands created to facilitate the analysis and interpretation of the hydrochemical data. C) Example of the Query form created as a user-friendly

application for different spatial-temporal queries on the hydrochemical data stored in the geospatial database.

#### 4.2.2.1 Spatial database.

The geospatial database (HYDOR) represents information based on the Personal Geodatabase structure provided by the ArcGIS concept. A Personal Geodatabase (Ormby et al., 2010) is a Microsoft Access database that can store, query, and manage a vast multiformity of data such as attribute data, geographical features, satellite and aerial images (raster data), CAD data, surface modeling or 3D data, utility and transportation network systems, GPS coordinates, and survey measurements. Furthermore, this structure is capable to apply sophisticated rules and relationships to the data and to define advanced geospatial models (e.g. topologies, networks, etc).

The GIS-based approach has proven to be an efficient tool for the implementation of a groundwater database in several hydrogeological studies (e.g. Gogu et al., 2001; Carrera-Hernandez and Gaskin 2008; Chesnaoux et al., 2011; Romanelli et al., 2012).

Although the database described here was implemented within ArcGIS, most of these concepts are sufficiently flexible to enable implementation in other GIS software or non-spatial databases.

# I. <u>Data content</u>

The hydrogeological database is composed of different datasets that store a variety of key spatial and non-spatial data necessary for a complete Hydrogeological study.

The main components include geographical (e.g. Digital Elevation Models), hydrogeological (e.g. well descriptions, springs, head measurements, extraction measurements), hydrological (e.g. river, lakes, wetlands), environmental (e.g. vulnerable or protected areas, soil uses), geological (e.g., lithology, stratigraphic units, depth to bedrock), geophysical (e.g. diagraphy), hydrometeorologycal (e.g. precipitations) and administrative features (e.g. owner, administrator).

In order to ensure the standardization and the harmonization of the data, several libraries (e.g. list of lithology, type of wells, units) were created, taking into account standard guidelines like the INSPIRE (INSPIRE, 2013) or the ONEGeology project.

A complete description of this database falls beyond the scope of this paper (for further information see Velasco et al 2012b and Velasco et al, 2013b). However, further details of the components of the database directly related to hydrogeochemistry and the main characteristics of its structure are given below in order to better illustrate the current platform. A sketch of the components of the database can be visualized in Figure 4.2.

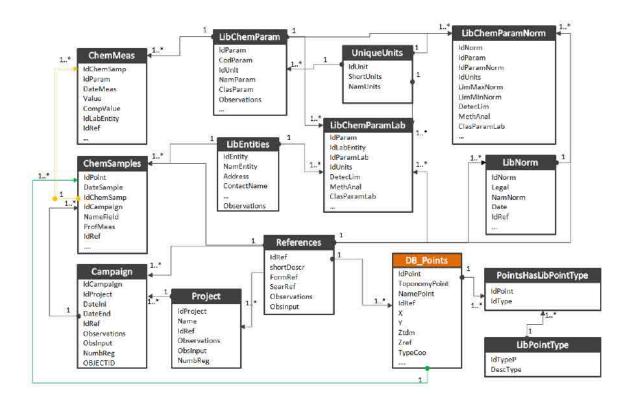


Figure 4.2. Simplified conceptual diagram representing the main contents of the hydrogeochemical database. The 1 and 1\*.. represents the cardinality of the relationship between tables.

In the hydrogeological database, each hydrogeochemical sampling site is correctly represented by a point-type entity. The main attributes of this are the geographical coordinates with a description of the different names used to identify those points of information (potential different sources of data) point accessibility, and other administrative information. Besides, other attributes that depend on the type of sampling point are added in further tables (e.g. wells, springs, rivers, etc).

In regards to the parameters measured for each sample, the database allows the entry of physico-chemical data stemming from both laboratory results and in situ measurements. The database enables the introduction of organic and inorganic compounds, including different isotopes. In addition, parameters such as temperature, Eh, pH, Electrical Conductivity (EC), alkalinity, etc are registered. Further information about existing standard regulatory guidelines is also included. Consequently, the hydrogeochemical data can be classified according to the threshold approach established by a given norm. The hydrogeochemical measurements made at each sampling point are stratified within the database in accordance with campaign, sampling date, name and depth. Thereafter, each sample is stratified in accordance with sampling data analysis, parameter, value and units of measurement.

Besides, other relevant information such as the characteristics of the measurement site, in situ methodology of measurements, analysis protocol, classification and detection limits for

different laboratories and information about the campaign can be readily included in the database. Finally some hydrochemical validation checks are performed to ensure consistency.

#### II. Computing and recording the data

As for data insertion, the management system of the geodatabase enables importing information coming from different formats such as spatial or non-spatial databases or spreadsheets. Furthermore, different forms are available for "one to one" or "massive data". Digital data (other database or spreadsheets) can be transferred to the geospatial database through the use of intermediate conversion tables. Otherwise, if the data are hand written, they should be introduced manually using assisted menus following an entry protocol.

Data controls to avoid errors when introducing data and to improve the harmonization and the analysis of the hydrogeochemical data were developed. For instance, a permissible value list was introduced to facilitate the encoding of physical and chemical parameters.

Also, other utilities to facilitate the conversion of measurement units were developed to avoid inconsistencies in the units of measurement between different data sets.

### III. Querying the data

To facilitate data retrieval and expedite the spatial analysis process of the hydrogeochemical data, a series of GIS-based tools and other specific query forms were developed and will be discussed below (sections 4.2.2.2 and 4.2.2.3). Additionally, other spatial and non-spatial queries may be generated from the geodatabase by using the inherent capabilities of ArcGIS and/or by using the standardized MS Access query builder.

# 4.2.2.2 Spatial Quimet

This includes a set of GIS-based tools that provide specific query forms using multiple search criteria for consulting, pre-processing and interpreting the hydrogeochemical data stored in the database. The tools were developed as an extension of the ArcMap environment, which is part of the ArcGIS v.10 software packages. They were created with ArcObjects, a developer kit for ArcGIS based on Component Object Model (COM), and programmed in VBPL using the Visual Studio (2008) environment.

The advantages of customized components by using a COM-Compliant environment such as Visual Studio are (ESRI, 2004; Boroushaki and Malczewski, 2008; Rahman et al., 2012): (1) a great range of functionalities can be integrated into customization; (2) codes are not accessible by the user; (3) all aspects of ArcGIS application can be extended and customized; and (4) the customization can be easily supplied to the client machines.

This extension has the form of a toolbar integrated into the ArcMap environment (See Figure 4.1) and consists of the following instruments: (I) Parameter calculator tools, (II)

Hydrochemical diagram tools, (III) Hydrochemical data analysis tools, (IV) Regulatory parameter analysis tools, and (V) Edition Hydrochemical data tools.

Additionally, ArcGIS inherent commands such as select by rectangle and add data together with the entire menu of the extension of Geostatistical Analyst are integrated into the same customized toolbar automatically.

#### I. Parameter Calculator Tool

This tool consists of a query form (see Figure 4.3) that allows the user to perform the following tasks for a pre-selected dataset:

- Calculate charge balance error (CBE) of chosen chemical analysis stored in the database. If one of the major ions is not available this computation cannot be performed.
- Automatically converts the units of the major elements to miliequivalent per litre (meq/l) and calculates the relative content of a cation or anion as a percentage of total cations and anions.
- Performs calculations such as the ionic relationship of the pair of species constituted by Na/K, Mg/Ca, SO4/Cl and Cl/HCO3, the icb index (disequilibrium chlorides and alkaline index) and the SAR index (sodium adsorption ratio).
- The results of such queries are displayed in a customizable table that contains all the aforementioned calculations or can be exported into MS Excel or MS Word.

The selection of the hydrochemical data to be analyzed is performed in two steps. The first step is to select a point or a set of points on the screen that represents sampling sites (e.g. **GwPoints**). This can be done by using any of the available select commands (e.g. select by location or by rectangle) of ArcMap, or else the command already integrated into the toolbar. Thereafter, the user selects the period of time of sampling that he/she wishes in the query form. Additionally, the user can also obtain the aforementioned calculations for different periods of time for a given sampling point.

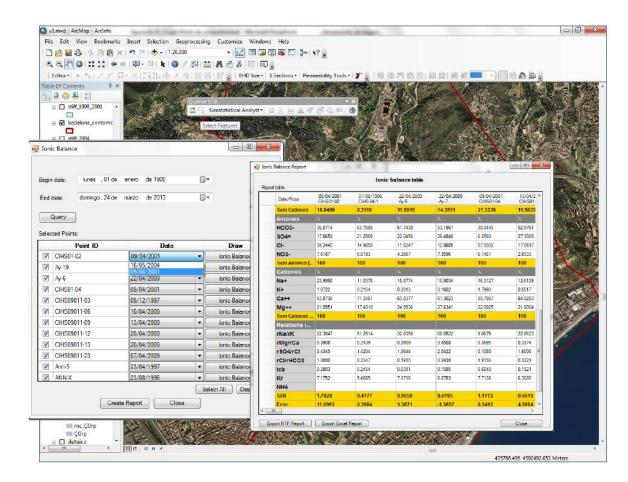


Figure 4.3. Example of a query form with the corresponding results of the command Parameter Calculator Tools.

# II. <u>Hydrochemical diagram tools</u>

This set of tools (represented by different buttons in the toolbar) was designed to facilitate the creation of standard hydrogeochemical diagrams for interpreting groundwater chemical analysis. Piper, Salinity diagrams, Schöeller-Berkaloff, and Modified Stiff diagrams can be created automatically for the chosen dataset (only if the parameters necessary for the creation of each diagram are available).

As occurs with the parameter calculator tools, the selection of the data is done by selecting a point or various points in the map for a given period of time. Additionally, the diagrams can also be obtained for a given point for different intervals of time. The resulting diagrams and the attached information (tables with the concentration values expressed in meg/l of each component) can be visualized on the screen or can be exported to MS Word.

The Stiff diagram is probably the most widely used to display the variation of several ions in the same map. However, where high variability exists in major ion concentrations, a tool to harmonize the size displayed in the map is necessary (Lee, 1998). For this reason, the

representation of the Stiff diagram in the map can be customized by the user by choosing diverse concentration scales.

Figures 4.4, 4.5 and 4.6 show some of the functions of this module.

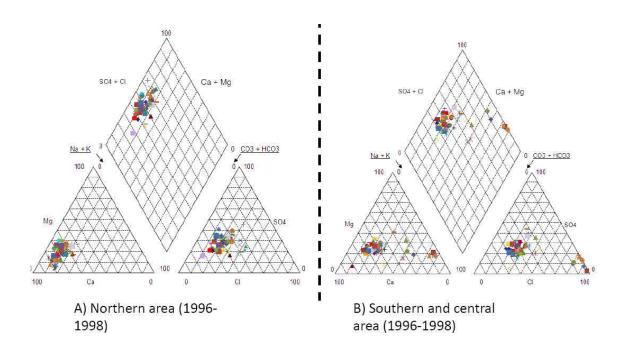


Figure 4.4. Piper diagrams obtained by using the command Hydrochemical diagram tools of the Spatial QUIMET module for the period 1996-1998 and corresponding to two subareas: A) northern area, B) central and southern area of the shallower aquifer.

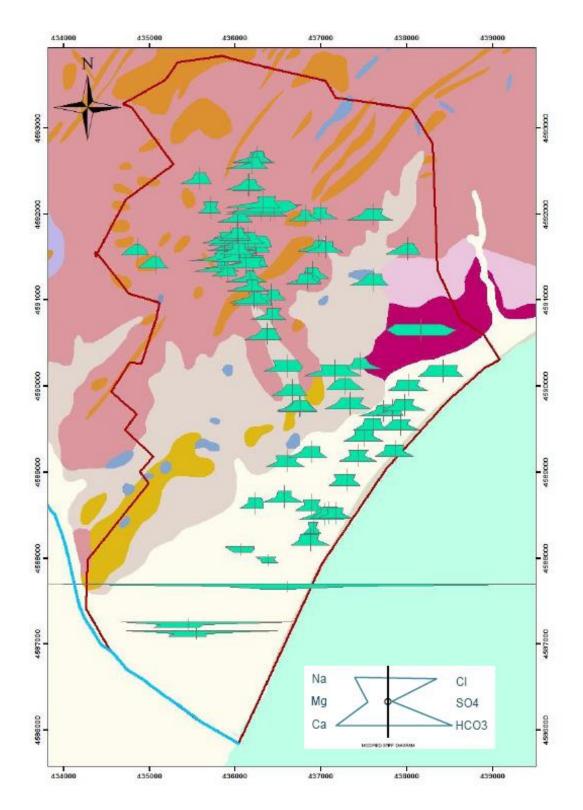


Figure 4.5. Map representing the Stiff diagrams of the Badalona shallower aquifer for the period 1997-2001. This map was elaborated with the command Hydrochemical diagram tools.

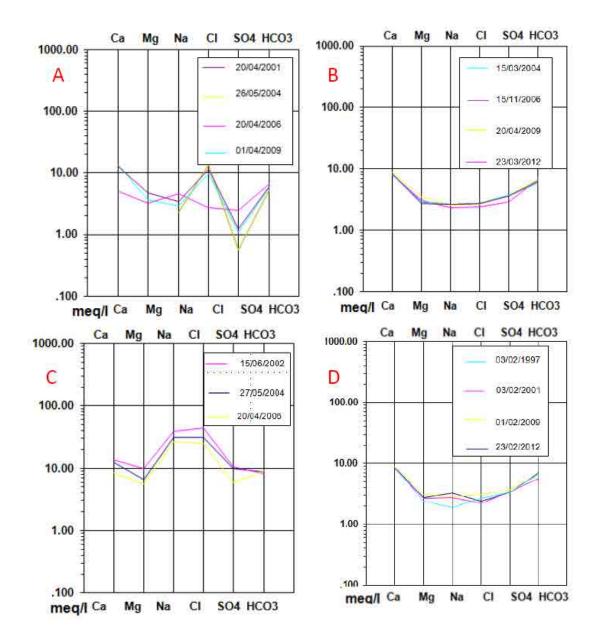


Figure 4.6. Schöeller-Berkaloff diagrams for 4 different points distributed over the study area (see the location of sampling points in figure 4.11).

# III. <u>Hydrochemical data analysis tools</u>

This instrument enables us to use the following range of methodologies and calculations for querying, interpreting and comparing groundwater quality parameters:

 Data Query. As shown in Figure 4.7 the query form enables the user to apply one or several query criteria (sampling point, campaign, time interval, parameter, etc) and to combine them for advanced queries on the hydrogeochemical data stored in the geospatial database. Results of the query are displayed in a list form where the user can also select the data for further

- queries (see below), or else can be exported to MS Excel for further calculations or to a MS Word file.
- Creating maps. This tool enables calculating the minimum, maximum, average
  and standard deviation for each selected parameter, for a given period of time
  and for a point or a group of selected points, and to represent these values in
  a map as shapefiles (the number of samples used is also displayed in the map).
  Results can be easily used for further geoestatistical analyses in the same
  ArcMap environment (using geostatistical analyses tools already integrated
  into the toolbar), or in other external platforms.
- Plotting graphs. This command explores whether correlations exist between two or more chemical elements, generating plots where the temporal component is also added.
- Link to EASYQUIM. This command enables us to retrieve the information and perform calculations for the selected points and data intervals. This is based on program EASYQUIM a free software developed as a plug-in in MS Excel (thus offering to the user a great portability) to draw traditional graphical methods and to compute a number of indices that are useful for hydrogeochemical data interpretation. Consequently, the user obtains in a portable format the following diagrams: Piper, Salinity diagrams, Schöeller-Berkaloff, and Modified Stiff diagrams, as well as tables for CBE, icb index and SAR index or ionic ratios.
- Link to MIX. This command allows obtaining the necessary information for the
  calculations with the MIX code for selected points and time intervals. MIX
  allows the evaluation of mixing ratios using the concentration of mixed
  samples assuming that the samples are a mixing of recharge sources (or end
  members) in an unknown proportion. The dating of this procedure is still ongoing.

# IV. Regulatory parameter analysis tool

This tool allows the user to obtain thematic maps for the parameters measured in the queried area classified according to the threshold approach established by a given guideline or just chosen by the user. This allows the identification of areas where determined chemical species exceed some specified limit (see Fig. 4.8).

# V. <u>Hydrogeochemical data Edition tools</u>

This utility enables visualizing and editing the attached information of a given point by selecting it in the map (see Fig. 4.9). As a result, the user can consult and edit (if necessary) the type of sampling site (e.g. well, lake, river) and the measurements available at this point (data of sampling, parameters, etc).

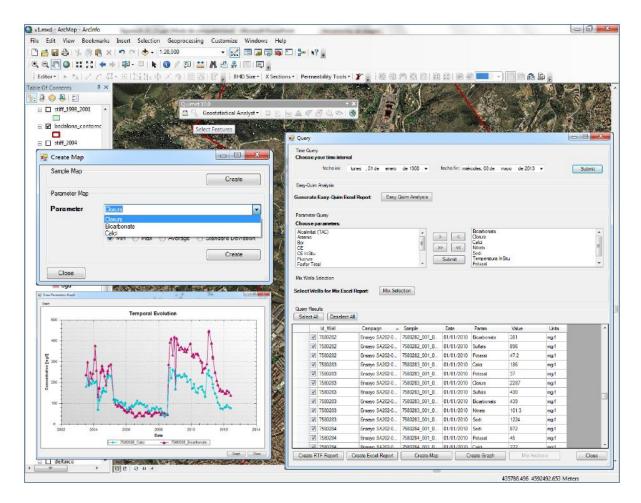


Figure 4.7. Example of a query form with the corresponding results of the command Hydrochemical data analysis tools.

#### 4.2.2.3 Statistical QUIMET

This set of instruments enables the user to perform a complete statistical analysis of the data. As occurs with the spatial analysis tools, it offers a query form that allows us to choose a time interval and the set of parameters to be queried. Furthermore, the user can easily query the entire time series for one or more parameters (see Fig. 4.1).

The result of this query is automatically exported to an Excel spreadsheet containing information on the samples where the requested parameters have been collected during the specified time interval. By using a set of commands, the user can perform the following calculations:

• Descriptive statistical analysis. This command calculates the following statistical parameters from univariate analysis: mean, standard deviation, variance, minimum, maximum, kurtosis, quartiles (25%, 50%, 75%), and skewness coefficient. It also creates scatter plots, histogram, and box plots.

- Parameter correlation Matrix. Generates R2, correlation and covariance matrices of the selected parameters.
- Bivariate analysis. This command produces correlation graphics for each pair of selected parameters.

Although this module operates independently of ArcGIs, the results obtained here may be exported to ArcGIs to perform additional analyses. Moreover, those result obtained with the *Hydrogeochemical Analysis tools* (see section 4.2.2.2) can be processed here for a more complete statistical analysis.

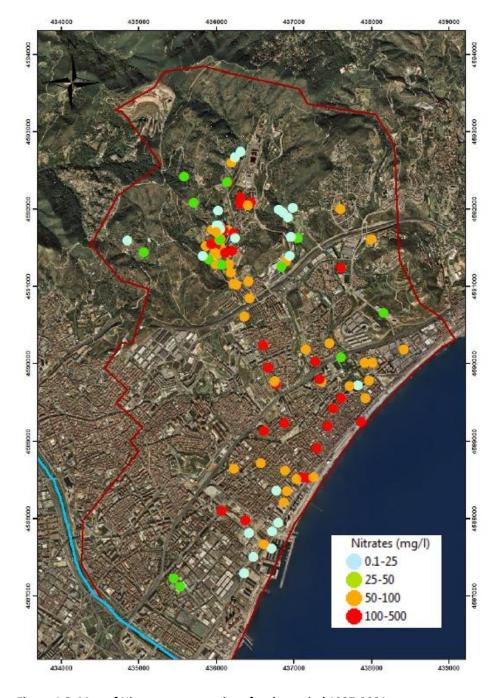


Figure 4.8. Map of Nitrate concentrations for the period 1997-2001.

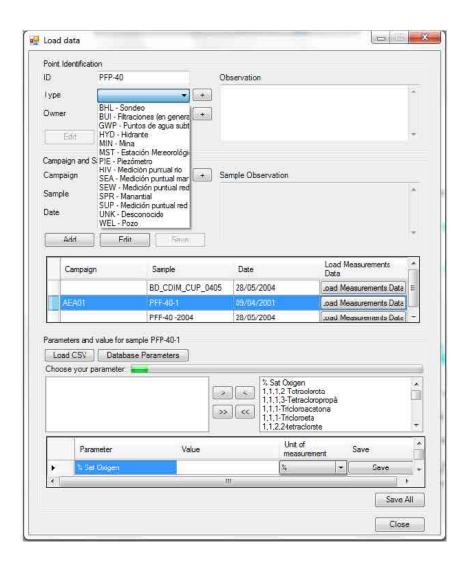


Figure 4.9. Query form of the command Edition Hydrochemical data tool.

# 4.3 Application

The QUIMET software platform was used in a case study involving a urban aquifer to illustrate its application. The study area is located in Badalona, a highly urbanized area on the Mediterranean coast in the north-eastern Spain (see Figure 4.10). Geologically, the study area is characterized by the presence of Quaternary deposits that deposited over a Paleozoic and Cenozoic rocks (Figure 4.11). The main features of the geological units in this area are summarized in Table 4.1 (for further information see Vázquez-Suñè et al., 2005a; Casatmijana et al., 2001; Velasco et al., 2012a).

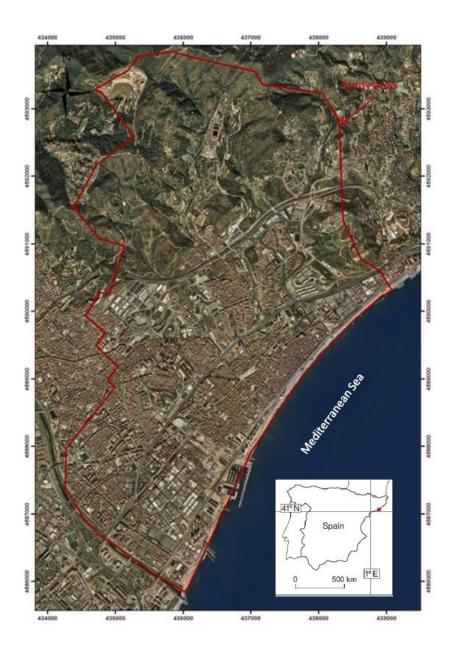


Figure 4.10. Ortograph of the study area that correspond with Badalona Drainage Basin. Coordinates are in Universal Transverse Mercator (UTM), zone 31.

In this area, different aquifer units with individual sedimentological, petrophysical and morphological characteristics (table 4.1) can be distinguished. Three areas may be differentiated: northern, central and southern. The northern and the central areas can be represented by a single aquifer whose hydraulic parameters depend on the permeability and thickness of the detritic units in the central part (mainly alluvial and fluvial deposits). The southern area is covered by deltaic and litoral deposits (mostly sandy gravel deposits) which constitute three aquifers separated by two lutitic units that wedge towards the margins.

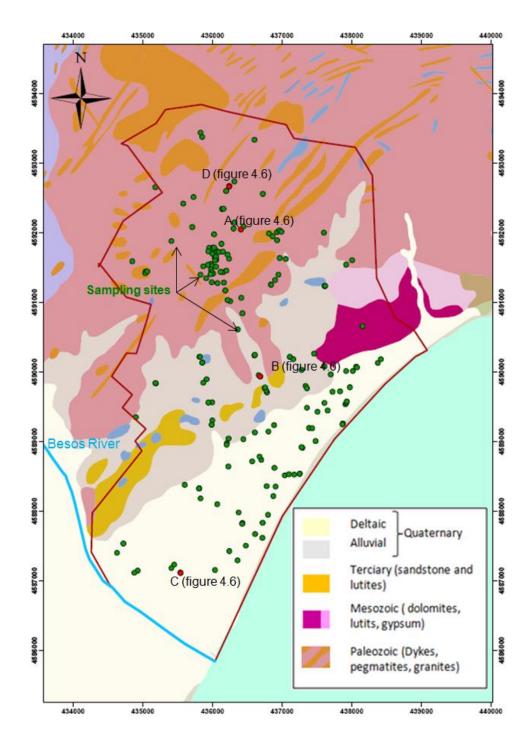


Figure 4.11. Geological map of the Badalona Drainage Basin provided by IGC (Geological Survey of Catalonia) with sampling points in green. See also table 4.1 for further information of the geological settings of the study area.

These aquifers have been used as supply for domestic and industrial purposes in the last decades, posing a serious threat to the quantity and quality of the groundwater resources of the study area. Several hydrogeological characterizations have been made along the years to ensure sustainable and effective water management of these aquifers (Alcolea and Sanz, 2001;

Casamitjana, 2002; Vazquez-Suñe et al., 2005a; Mendez and Montes, 2009; Araya and Goyeneche, 2012), altogether providing a large data set, mainly concentrated in the shallow aquifers.

AGE		UNIT	LITHOLOGICAL DESCRIPTION	HYDROGEOLOGICAL DESCRIPTION			
Quaternary	Holocene	Fluvial Silty to slightly silty sands deposits with gravels		Partially permeable ( permeable in areas with less silt)			
		Alluvial deposits	Sandy silt with gravels	Less permeable ( only permeable in areas with less silt and clay)			
		Deltaic	Sandy gravels	Aquifer			
		deposits* *In the study	Gray clay and silts with some fine sand	Less permeable			
		area	Sandy gravels	Aquifer			
		Litoral deposits	Sand and gravels	Aquifer			
	Pleistocene	Alluvial deposits	Red silty sand with gravels	Partially permeable (only permeable in some areas with less silt and clay)			
Terciary	Upper Pliocene	Sandstone a and clayey r	and conglomerate with sandy matrix	Less permeable			
	Lower Pliocene	Grey marls					
	Miocene	Matrix rich	gravels and sandstone	Less permeable			
Mesozoic	Muschelkalk	Sequences of lutites and g	composed by dolomites, red gypsum.	Less permeable			
<u>IMESOZOIC</u>	Buntsandstein	Sequence for conglomera	ormed by sandstone and red ates	Less permeable			
Paleozoic	Ordovician	Shales		Less permeable			
	Hercinic	Granodiorit	es and aplites dykes	Partially permeable (in areas with fractures and weathering)			

Table 4.1. Lithological, hydrogeological and chronological description of the different geological units of the study area (after Montes et al., 2005 and Campo, 2004).

The geospatial database includes approximately 300 samples distributed over the study area over 202 points as shown in Figure 4.11. Data includes head measurements, geological description, meteorological information, and chemical analysis from samples taken between 1996 and 2012. Among the 110 hydrogeological variables in the compiled database (physical parameters, organic and inorganic species, isotopes), we selected only those with the highest frequency for a detail evaluation (EC, pH, and the following ions, Ca, Mg, Na, K, Cl, SO4, HCO3, PO4, NO3 and NH4).

The first step was to test the chemical analysis for charge balance (CBE) by using the Parameter calculator tool (section 4.2.2.2). In 93% of the samples CBE was less than or equal to  $\pm 10\%$ , an error found acceptable for the purpose of this study. Indexes such as SAR, icb and ion ratios were also calculated for each selected point by using this command.

The next step was to analyze the hydrogeochemical data by using widespread geochemical techniques including spatio-temporal representation of the data, correlations of different species, and graphical diagrams (Piper, Stiff, Schöeller-Berkallof). This was accomplished by using the different commands of the *Spatial Quimet Tools* (see section 4.2.2.2)

As a result, in the northern part of Badalona, which is mainly constituted by granite, the water can be classified as HCO3-Ca type (see Figures 4.4 and 4.5). In the southern and central areas the water can be classified as HCO3/Cl-Ca/Na type, probably as a result of cation exchange between sodium and calcium in the finer quaternary alluvial deposits and enrichment in Na and precipitation in Ca in the granitic structures. In the western area of the central part, the water becomes of SO4-Mg type owing to the presence of gypsum and dolomites in the Triassic units. This fact can be visualized in the Stiff maps obtained for the time period between 1996 and 2001 (Figure 4.5). Finally, at several points located in the south east (next to the Besòs Delta River and the coastline) the water shows a tendency to become of Cl-Na type, suggesting seawater intrusion probably produced by coastal aquifer overexploitation.

The electrical conductivity (EC) of the groundwater in this area normally ranges around 1000 uS/cm and its spatial distribution is fairly homogeneous for most of the time intervals consulted. Only at some points affected by seawater intrusion and urban contamination near the coastline and in some Triassic materials do the CE show values above 2000 uS/cm.

In general, spatial variability rather than the temporal factor is the most important source of variation in the data, demonstrating that groundwater chemistry is conditioned by the subsoil materials except in areas affected by contamination. Figure 6 displays Schöeller-Berkaloff diagrams for 4 different points distributed over the study area. These diagrams show that groundwater chemistry does not significantly change over time. Only at some points can a slight change be appreciated. For instance, in example A, the sulphate content shows an increase in 2006, whereas the chloride content decreases. In example C, theoretically affected by seawater intrusion, the concentration of the major elements decreases slightly between 2002 and 2006.

In order to evaluate the groundwater quality of the study area and to detect possible sources of contamination, several spatial distribution maps of a number of parameters were obtained by using another command of the Spatial Quimet tools (Hydrochemical data analysis tools). These maps (see Fig. 4.8) show that the content of components that usually indicate contamination caused by residual water such as nitrate and phosphate is higher in the urbanized areas except at some points affected by activities such as irrigation or livestock farming.

Besides this spatio-temporal analysis, further statistical analyses were performed by using the statistical QUIMET tools. For instance, several correlation matrices of 8 variables (EC and major elements) were calculated. The following tables shows two examples of two correlation matrix obtained for two groups of samples collected in the nortern and in the southern part of

the study area. It is found that the content of chloride is positively and strongly correlated with calcium in the northern area for the selected samples (see table 4.2), whereas in the southern area chloride is strongly correlated with sodium (see table 4.3).

	Bicarbonates	Sulphates	Chloride	Nitrates	Sodium	Potassium	Calcium	Magnesium	CE
Bicarbonates	1.00	0.19	0.16	0.01	0.38	0.13	0.30	0.31	0.35
Sulphates		1.00	0.06	0.56	0.29	0.30	0.42	0.50	0.46
Chloride			1.00	0.51	0.47	0.54	0.83	0.03	0.85
Nitrates				1.00	0.46	0.44	0.72	0.29	0.68
Sodium					1.00	0.48	0.35	0.38	0.60
Potassium						1.00	0.49	0.21	0.59
Calcium			0.83	0.72			1.00	0.04	0.87
Magnesium								1.00	0.31
CE			0.85	0.68	0.60		0.87		1.00

Table 4.2. Correlation matrix of the major ions and electrical conductivity (EC) for the selected group of samples in the northern part of the study area obtained by using the Statistical QUIMET module.

	Bicarbonates	Sulphates	Chloride	Nitrates	Sodium	Potassium	Calcium	Magnesium	CE
Bicarbonates	1.00	0.36	0.16	-0.04	0.23	-0.10	0.62	0.52	0.56
Sulphates		1.00	0.35	0.23	0.38	-0.14	0.48	0.62	0.62
Chloride			1.00	0.04	0.83	0.45	0.13	0.30	0.76
Nitrates				1.00	0.12	0.05	0.30	0.39	0.37
Sodium			0.83		1.00	0.53	-0.07	0.29	0.73
Potassium						1.00	-0.37	-0.01	0.22
Calcium	0.62						1.00	0.40	0.54
Magnesium		0.62						1.00	0.60
CE		0.62	0.76		0.73			0.60	1.00

Table 4.3. Correlation matrix of the major ions and EC of a group of samples located in the southern part of the study area obtained by using the Statistical QUIMET module.

# 4.4 Discussion and conclusions

The QUIMET software platform presented in this paper offers a user friendly GIS environment with a large variety of automatic tools developed specifically for the management and analysis of hydrogeochemical data to facilitate their interpretation.

One of the main elements of this platform is the geospatial database that enjoys the following advantages: 1) an effective management of a large number of different types of hydrogeological spatial-time dependent data, 2) the possibility of querying and visualizing data simultaneously, facilitating further data correlations and interpretations, 3) a synoptic view of the groundwater quality data and 4) an efficient pre-processing and pre-filtering of the hydrochemical data.

Even though the database schema here was implemented within a Personal Geodatabase (ArcGIS, ESRI), we note that it could also be implemented within other GIS and Spatial Relational Database Management System (RDBMS) software.

Despite the complexity of the internal structure of the database, the consultation of the data is simple using the different multi-criteria query forms. For instance, the Statistical Quimet Tools offer the user a complete statistical analysis of data, including descriptive statistical analysis, bivariate analysis, generation of correlation matrix and correlation graphics. Furthermore, the multi-choice query forms belonging to the Spatial Analysis Tools provide multiple queries for comparing temporal and spatial groundwater parameters. Additionally, useful calculations of hydrochemical parameters (e.g. ECB, ionic ratios, etc), thematic maps, plots with temporal evolution of parameters or preselected data for a further geostatistical analysis, can be easily obtained.

Moreover, this paper shows how it is possible to integrate a wide range of specific methodologies for hydrogeochemical analysis into a single GIS-based software platform. This includes the traditional hydrogeochemical diagrams (Piper, Stiff, etc) allowing the combination of several sampling points and campaigns to be analyzed in an integrated framework by automatically generating them using tools belonging to Spatial Analysis Tools.

QUIMET offers interoperability with other external platforms such as EASYQUIM or MIX. Moreover, with adequate adjustments this software platform could be readily linked to other programs such as PHREEQC or SGeMs, considerably increasing the variety of hydrogeochemical calculations.

# 5 A SEQUENCE STRATIGRAPHIC BASED GEOLOGICAL MODEL FOR CONSTRAINING HYDROGEOLOGICAL MODELING IN THE URBANIZED AREA OF THE QUATERNARY BESÒS DELTA (NW MEDITERRANEAN COAST, SPAIN)

# 5.1 Introduction

An adequate management of the groundwater resources under metropolitan areas is becoming increasingly important in scientific, economic, social, legal and political terms (Vázquez-Suñè, 2003; Kulabako et al., 2007). In numerous cases, human settlements are situated directly over sedimentary aquifers, the groundwater of which is used for industry and domestic consumption. In addition, the presence of water stored in the subsurface poses risks for civil engineering works (Bonomi and Cavallin, 1997; Vázquez-Suñé et al., 2005). In such scenarios, hydrogeological models that describe and predict flow and transport in the aquifer are of great benefit to an effective management of the subsurface (Pokrajac, 1999, Vázquez-Suñé et al., 2006, Carneiro and Carvallo, 2010). The complex nature of the process that controls the sedimentary media often produces a highly heterogeneous distribution of hydrogeological parameters in aquifers. In this regard, some authors (Huggenberger and Aigner, 1999; Klingbeil et al., 1999; Heinz et al., 2003; Sharpe et al., 2003; Ezzy et al., 2006), have highlighted the importance of constraining the models of flow and transport of solutes to the sedimentological heterogeneities of the aquifer. Nevertheless, defining the geological heterogeneities that control flow behaviour in sedimentary aquifers and especially, in those located under urbanized areas, is not easy. Outcrops, where they exist, are very limited and data are sparse and are derived from diverse sources, making a suitable integration and management difficult (Velasco et al., 2012b).

During the last decades, advances in hydrocarbon exploitation and in hydrogeology have gone hand in hand with the development and implementation of new technologies. In this regard, the development of three-dimensional models of subsurface heterogeneity has proved to be an efficient tool for the management of reservoirs in geological scenarios that are

This chapter is based on the paper Velasco, V., Cabello, P., Vázquez-Suñè, E., López-Blanco, M., Ramos, E., & Tubau, I. (2012). A sequence stratigraphic based geological model for constraining hydrogeological modeling in the urbanized area of the Quaternary Besòs delta (NW Mediterranean coast, Spain). geologica acta, 10, 373–394. doi:10.1344/105.000001757

[Chapter 5: A sequence stratiraphic based geological model for constraining a hydrogeological model in the Besòs Delta (NW Mediterranean coast , Spain)]

practically inaccessible and where data are limited (Matheron et al., 1987; Gundeso and Egeland, 1990; Stanley et al., 1990; Weber and van Geuns, 1990; Bryant and Flint, 1993; Krum and Johnson, 1993; Deutsch and Hewett, 1996; Dubrule and Damsleth, 2001) and for the management of water resources (Ross et al., 2005; Robins et al., 2005; Lelliot el al., 2006; Robins et al., 2008). In reservoirs and aquifers in sedimentary media, the distribution of petrophysical properties that control flow is closely linked to the distribution of depositional facies.

Thus, a general 3D workflow modeling of sedimentary reservoirs and aquifers involves the modeling of facies distribution at an early stage to constrain flow models. Facies models are based on the depositional model for the reservoir or aquifer and describe the sedimentary heterogeneity at multiple scales. This is a critical point in the modeling process as flow predictions are highly dependent on facies heterogeneity (Falivene et al., 2006; Howell et al., 2008; Cabello et al., 2010). This workflow modeling is of paramount importance to an effective management of the aquifers of highly urbanized areas in Quaternary deltas since such formations usually act as aquifers owing to their geological (i.e. sedimentological, petrophysical and geomorphological) characteristics (Gámez et al., 2009). An example of aquifers situated under large urbanized areas is found in two deltaic formations located in the metropolitan area of Barcelona, on the Mediterranean coast in NE Spain. This very densely populated area is located on the Llobregat and the Besòs Holocene deltas (Fig. 5.1). This urban region, with more than 2 million inhabitants, has an active underground infrastructure, which is threatened by the presence of water in the upper meters of the two deltaic aquifers. In addition, the aquifers in the Llobregat and the Besòs deltas have been used as a water supply for domestic and industrial purposes in the last decades, which pose a serious threat to the quantity and quality of groundwater resources. Finally, given the possible continuity of the aquifers seawards and the possible connection to the sea, a sound knowledge of geology and hydrogeology both onshore and offshore is necessary to forestall marine intrusion (Abarca et al., 2006; Gámez, 2007). The need to understand aquifer behavior for an effective management has prompted the scientific community to study the geological and hydrogeological characteristics of both deltas (Marqués, 1974, 1984; Manzano, 1986; Vázquez-Suñé et al., 2005; Lafuerza et al., 2005; Gámez, 2007; Gámez et al., 2009; Riba and Colombo, 2009). As regards the Besòs delta, a number of hydrogeological studies have been carried out during the last century. These works include Moragas (1896), Rubio and Kinderlán (1909), the hydrogeological synthesis study carried out by the Ministry of Public Works of Spain together with the Hydrographic Confederation of Eastern Pyrenees (MOP, 1966) in addition to more recent studies of Nilsson et al. (2002) and Ondiviela et al. (2005). Nevertheless, given the implications for human activity, much more research is needed to improve our understanding of deltas and the management of their aquifers. The present paper seeks to upgrade hydrogeological modeling in deltaic depositional systems by focusing on the benefits obtained from modeling detailed subsurface geological heterogeneities. The Besòs delta was chosen as the example for this purpose. The workflow modeling and results in this chapter are presented as follows: i) a summary of the database used for the characterization and modeling of the [Chapter 5: A sequence stratiraphic based geological model for constraining a hydrogeological model in the Besòs Delta (NW Mediterranean coast , Spain)]

Besòs delta; ii) the integration and synthesis of these data that enabled us to define facies association and sequence stratigraphic arrangement of the sedimentary record onshore and offshore; iii) a three-dimensional model reproducing distribution of facies associations in the Besòs delta, based on geological characterization (i.e., facies belt and stratigraphic organization) and iv) a consistent hydrogeological model constructed on the basis of the three-dimensional geological model. The hydrogeological model was calibrated by historical data of water management and production of the last century to constrain and revise parameters used in the modeling process.

# 5.2 General setting

# 5.2.1 Besòs delta complex

The Besòs delta is located on the Mediterranean coast in the NE of the Iberian Peninsula (Fig. 5.1). It is an asymmetric, small delta that occupies an area of 17.4km<sup>2</sup> (Riba and Colombo, 2009). The Besòs delta is limited by the Littoral Ranges to the north, and by the Barcelona Coastal Plain to the west, which separates the Besòs delta from the neighbouring Llobregat delta (Figs. 5.1, 5.2). It is a Holocene depositional system that was also active during the Pleistocene. The delta is being constituted by sediments supplied by the Besòs River and their tributaries. The accumulated watercourse length of these rivers is about 530km and their drainage area is approximately 1038km<sup>2</sup> (Devesa et al., 2004). The present day Besòs River displays a very low sinuosity in its lower course and has been subjected to growing pressure from anthropic activities. The irregular hydrology of the Besòs River is characterized by an alternation between long periods of drought and catastrophic flows (Riba and Colombo, 2009). The upper Besòs delta plain slope is relatively high, about 0.2º (0.35% after Sanz, 1988) and the ratio of the submerged deltaic area to the emerged deltaic area is below 2 (Serra et al., 1985). The Besòs delta can be considered as an encased delta complex dominated by waves and longshore drift with coalescing minor alluvial fans derived from both margins. The Quaternary succession of the Besòs delta, which reaches a maximum thickness of 53m onshore and approximately 50m offshore (at 5km from the coastline), rests unconformably on a paleorelief (paleovalley) over a substratum formed by Paleozoic and Cenozoic rocks (Fig. 2). The Paleozoic lithologies are mainly slates and granites. The Cenozoic units are made up of Miocene matrix-rich gravels and sandstones, and Pliocene grey massive marls. As in the case of the neighbouring Llobregat delta (Gámez et al., 2009), the Quaternary sedimentation of the Besòs delta was mainly controlled by glacio-eustatic sea-level changes and fault activity (Riba and Colombo, 2009)

#### 5.2.2 Dataset

The study area covers the whole emerged portion of the delta in addition to the submerged part 5km offshore. The intrinsic geological complexity of the subsurface in the study area in addition to the progressive and massive urbanization that accelerated in the 1960s necessitated the compilation of geological information from a wide variety of sources (i.e. geological maps, geotechnical and hydrogeological perforations, etc.) both public and private. This dataset comprises: 372 boreholes of diverse origin (Fig. 5.3, 5.4); digital terrain models from the Institut Cartogràfic de Catalunya (ICC), 30x30m of resolution; a geological map of the Besòs delta and adjacent zones at 1:50,000 scale from the Instituto Geológico y Minero de España (IGME) (Alonso et al, 1977), and the Institut Geològic de Catalunya (IGC) (IGC-IGME, 2005); a geotechnical map of Barcelona at 1:25,000 (ICC, 2000); two seismic profiles from the IGME produced in 1989 (Medialdea et al., 1989) (see location in Fig. 5.3); and a compilation of bibliographic studies comprising references dating back more than a hundred years (Llobet and Vallllosera, 1838; Cerdà, 1855; García Faria, 1893; Moragas, 1896; Almera, 1894; Almera and Brossa, 1900; Rubio and Kindelán, 1909; Solé i Sabarís, 1963; Garau, 1983; Sanz, 1988; UPC et al., 1997; Montes and Vàzquez-Suñé, 2005; Simó et al., 2005; Adif, 2007; Gámez, 2007; Liquete et al., 2007; Martí et al., 2008; Gámez et al., 2009; Riba and Colombo, 2009). Additionally, extra fieldwork and aerial photographs interpretation of the Besòs delta were carried out for the elaboration of this work. The information was introduced into a geospatial database that integrated all the available data into a coherent and logical structure that enabled us to define a conceptual depositional model of the Besòs Delta on the basis of sequence stratigraphic analysis. The structure of this database also allows us to store several interpretations and models derived from the data (Velasco et al., 2012b and Velasco et al., 2013b).

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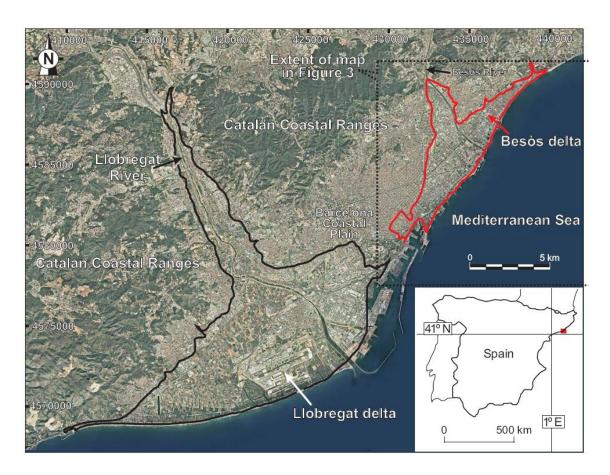


Figure 5.1. Orthophotograph of the northeastern Mediterranean coast of Spain covering the extent of the Besòs and Llobregat emerged deltas (see red point in lower right inset for general location). Both deltas are separated by the Barcelona Coastal Plain, and are bounded by the Catalan Coastal Ranges to the north (see the Geological map of this zone in Fig. 5.2). Note the intense urbanization of this region, hindering outcrop existence. Coordinates are in Universal Transverse Mercator (UTM), Zone 31.

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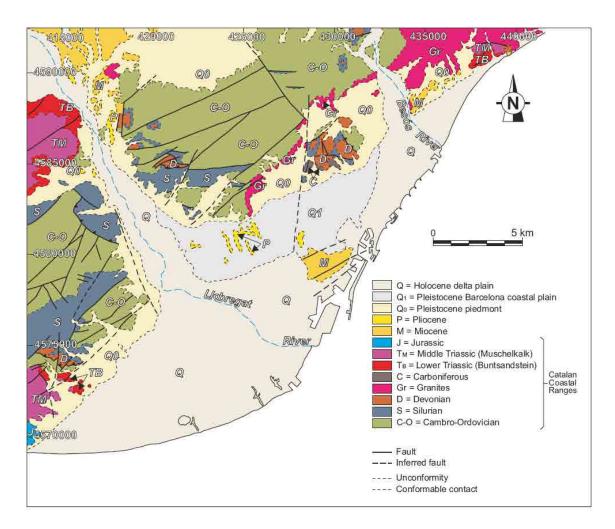


Figure 5.2. Geological map of the Besòs and Llobregat deltas, and adjacent zones (see the corresponding orthophotograph with the extent of the emerged deltas in Fig. 5.1).

# 5.3 Facies and sequence stratigraphic analysis

# 5.3.1 Sedimentary facies belt

In the Besòs Delta, the whole range of deltaic depositional environments (from continental to marine) was identified. In addition, several facies associations were defined within each depositional environment in accordance with the grain size distribution and sedimentary features such as fauna, roundness, sorting, etc:

# I. CONTINENTAL ( SUBAERIAL):

#### a. Proximal alluvial fan:

This facies association consists of deposits of heterometric gravels interbedded with sands and red-yellow muds. It is restricted to the areas where the Besòs Delta Complex is closer to the surrounding reliefs (*i.e.* the Littoral Coastal Ranges and the Barcelona Coastal Plain; Figs. 5.1, 5.2) and represents small-scale alluvial fan and screes derived from these reliefs.

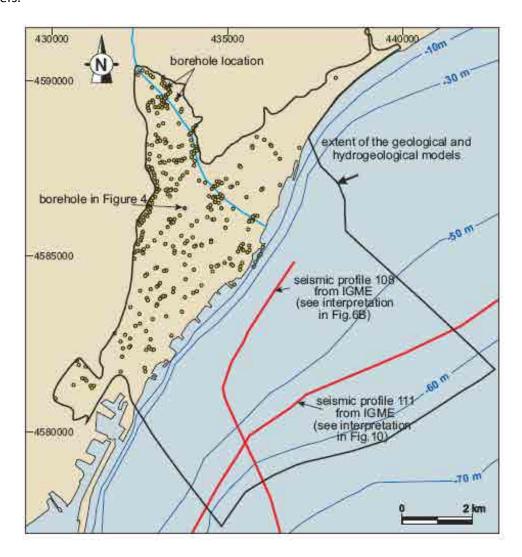


Figure 5.3. Schematic map showing the location of the boreholes used for the stratigraphic correlation and the geological modelling (see an example of a borehole interpretation in Fig. 5.4); the location of part of two seismic profiles, on which the stratigraphic correlation in the submarine part of the delta was based (see interpretation of seismic profile 108 and profile 111 in Fig. 5.6 and 5.10); and the extent of the geological and hydrogeological models. Note that the models presented cover the whole emerged portion of the delta (see Fig. 5.1), and extend five kilometres seawards from the coast including a portion of the submarine part.

#### b. Fluvial Channel:

This facies association consists of poorly sorted gravels with occasionally sandy matrix with some lenses of organic matter. The pebbles are well to poorly rounded, heterometric and polymictic. These deposits are capped by or are intercalated with the floodplain facies. This facies association is interpreted as deposits from fluvial channels and ephemeral fluvial courses. It commonly has great lateral continuity and may fill abandoned paleochannels.

# c. Floodplain facies:

This sedimentary facies association is composed of continental red and yellow clays and silt intercalated with coarser-grained deposits. It is interpreted as the distal alluvial fan and river floodplain deposition during flooding events. It laterally grades to a proximal alluvial fan towards the margins of the deltaic complex and it is commonly intercalated with fluvial channel deposits. It grades from distal to coastal facies.

### II. TRANSITIONAL:

Within this sedimentary depositional environment, two facies associations, which constitute the transgressive delta front and the regressive delta front of the deltaic system, were interpreted.

# a. Transgressive delta front:

This facies association is composed of a fining and deepening- upward succession of gravels (well rounded to angular pebbles) and sand with abundant marine fauna. It is interpreted as a reworking of alluvial and fluvial deposits by marine processes and is located on top of fluvial channels. The transgressive delta front is capped by prodelta clay and silts.

#### b. Regressive delta front:

This facies association consists of coarsening-upwards sandy units grading into gravels with abundant micaceous minerals and some shell fragments. It is interpreted as being the product of the progradation of the Delta front. It grades to fluvial channels and to floodplain upwards and to the margin.

# III. MARINE:

#### a. Prodelta:

Within this depositional environment one facies association comprising gray clays and silts with intercalations of fine sands and sparse marine fauna were identified. This association is interpreted as the Prodelta of the deltaic complex deposited below the storm wave base.

The Prodelta facies belt is located in the SE of the delta and grades to the delta front to the NW.

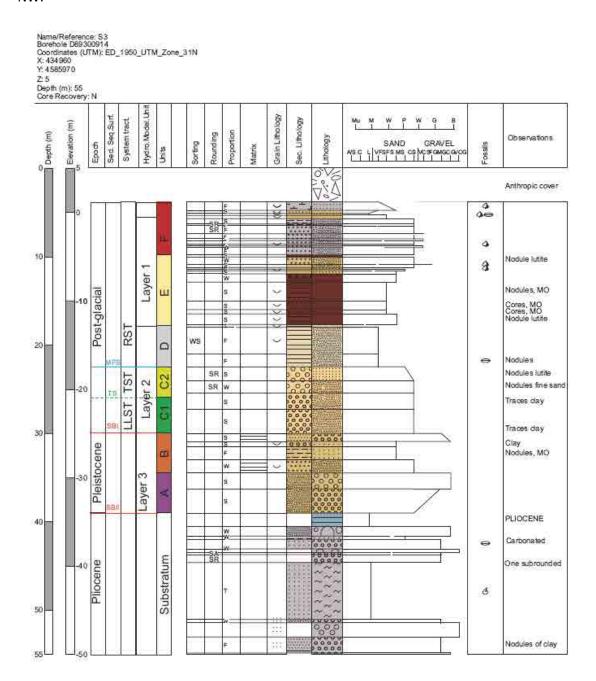


Figure 5.4. Example of a borehole interpretation from dataset compiled and used for the stratigraphic correlation and the geological modelling. The lithology is defined by three components: Lithology (main lithology), secondary lithology and matrix. The proportion between the secondary and the main lithology is represented by the column labelled as Proportion. The seven geological units distinguished, the stratigraphic surfaces, the system tracts, and the hydrogeological units of the model are indicated. Units A and B are included in the Pleistocene sequence, whereas units C1, C2, D, E and F correspond to the Postglacial upper sequence.

# 5.3.2 Sequence stratigraphic subdivision

Coastal and deltaic successions usually develop complex architectural arrangements owing to their sensitivity to relative sea-level changes. This type of complex architecture is governed by the relationship between accommodation (subsidence+eustasy) and sediment supply. Given that this case study deals with present-day and recent delta deposits, eustatic variations played an important role in their architectural development, as in other recent Mediterranean delta systems (e.g., Somoza et al., 1998; Montaner and Solà, 2004; Gámez et al., 2009).

Because this architectural arrangement was influenced by sea level changes, a sequence stratigraphic analysis of the Besòs delta succession is necessary to differentiate a series of sequences, systems tracts and key surfaces. This differentiation is useful to correlate boreholes, to predict depositional (and granulometric) trends and to forecast the geometry of the main facies belts in order to build a robust geological model.

The estimated ages are based on the comparison with depositional architectures described in other Mediterranean delta plains and shelves (*e.g.* Llobregat Delta, Ebro Delta) (Gámez, 2007; Gámez *et al.*, 2009).

The geological model of the Besòs delta in this study is based on a sequence stratigraphic subdivision. This subdivision resulted from the identification of key stratigraphic surfaces and the general trends (progradational-retrogradational or coarsening/fining upwards) observed in the marine and transitional sediments in the boreholes.

After the identification of the key surfaces and the different system tracts within the boreholes, these sequence stratigraphic units and key surfaces were correlated along several correlation panels covering the entire delta complex.

The delta was subdivided into two sequences, with thicknesses in the order of tens of meters, bounded at the base by widespread erosional surfaces (even paleoreliefs; Fig. 5). These erosional surfaces represent periods of subaerial erosion, probably related to relative sea-level falls associated with glacio-eustatic sea-level variations during the Quaternary. An accurate study of the coastal and marine facies succession is necessary to establish a reliable sequence stratigraphic subdivision. In this case study, the lower stratigraphic unit between two erosional surfaces is mainly constituted by continental sediments (Fluvial facies association and floodplain facies association). Owing to the lack of information about the sequential trends of time-equivalent marine and transitional deposits, an internal sequence stratigraphic subdivision in systems tracts was not developed.

The uppermost sequence embraces the whole range of facies belts (from subaerial to submarine) and a series of key surfaces and systems tracts have been defined. This sequence consists of: a) a lower late lowstand systems tract (Posamentier and Allen, 1999), b) a

transgressive systems tract (Van Wagoner et al., 1988), and c) an upper regressive systems tract (Embry and Johannessen, 1992).

The late lowstand systems tract is identified by fluvial channels resting above the erosive surface (*i.e.* sequence boundary; Fig.5.5). These channels were deposited during an initial relative sea-level rise after a sea-level fall, filling the erosive reliefs developed during the sea-level fall.

The transgressive systems tract is constituted by reworked channel facies association (Transgressive delta front). The basal surface is a transgressive surface, interpreted as a waveravinement surface, and is characterized by a gravelly lag derived from the reworking of late lowstand systems tract fluvial channel deposits during transgression. The top surface is a maximum flooding surface that in well logs was traced directly over a lithological change, recording an abrupt deepening of the water lamina reflected in prodeltaic sediments. The maximum flooding surface marks the change from fining/deepening-upwards to coarsening/shallowing-upwards vertical trends and also the change from retrogradational to a progradational arrangement in the delta front facies belt.

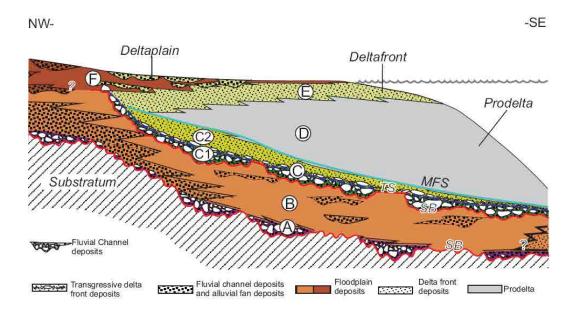


Figure 5.5. Synthetic cross-section showing the stratigraphic organization of the Besòs delta. Two widespread erosional surfaces, i.e. sequence boundaries (SB), subdivide the delta succession into two sequences: the lower Pleistocene sequence and the upper Postglacial sequence. In the Postglacial sequence, three systems tracts are distinguished: a lower late lowstand systems tract, in between the sequence boundary and a transgressive surface (TS); a transgressive systems tract, bounded by the transgressive surface and a maximum flooding surface (MFS); and an upper regressive systems tract above the maximum flooding surface. This sequence stratigraphic subdivision was correlated seawards with previous descriptions and interpretations of the submerged delta (see seismic profile interpretation in Fig. 5.6). The sequence stratigraphic surfaces and additional lithostratigraphic boundaries allowed to distinguish seven geological units (A to F), which present different sedimentological, and thus petrophysical and hydraulic properties (see Table 5.1 and 5.2 for more details).

The regressive systems tract shows coarsening and shallowing upwards trends (from prodelta marly clays and silts to delta front sands and gravels) and displays a progradational stacking pattern.

According to Garriga (2007), the arrangement of the Besòs delta is similar to the one described by Gámez *et al.* (2005) for the neighboring Llobregat delta. It is reasonable, therefore, to assume that the sequential arrangement in the Besòs delta was controlled by absolute sea-level changes occurring during the Quaternary as described by Gámez *et al.* (2005, 2009) and Gámez (2007) for the Llobregat Delta. Thus, the development of the defined systems tracts and sequences was controlled mainly by absolute sea level variations and sediment supply. Consequently, the uppermost sequence, Postglacial in age, records the decelerating sea-level rise after the last glacioeustatic minimum. The lowermost sequence, which is of Pleistocene age, probably records the last complete glacioeustatic cycle.

The correlation of the proposed stratigraphic subdivision with previous descriptions (Medialdea et al., 1989; Gámez, 2007) of the subsumerged delta based on seismic profile interpretations and borehole correlations provides an overall framework for the quaternary stratigraphic architecture of the continental margins.

This correlation enables us to establish the following equivalents (see Fig. 5.6C): the regressive systems tract and the transgressive systems tract of the Postglacial sequence were found to be equivalent to unit Q4 proposed by IGME (Medialdea et al., 1989). The Postglacial late lowstand systems tract and its basal unconformity correspond to the late lowstand systems tract of unit Q3 and to the forced regression systems tract of unit Q2. The Pleistocene sequence is equivalent to the highstand and the transgressive systems tracts of units Q2 and Q1.

# 5.4 Geological and hydrogeological model

#### 5.4.1 Geological model

The Besòs models presented in this paper are concerned with the emerged part of the delta in addition to 5km of the submerged part (Fig. 5.3). Stratigraphically, the model includes the entire delta succession ranging from Pleistocene deposits at the base to the Present top surface with stratigraphic thicknesses between 7.5 and 53.5m onshore and about 50m (5km from the shoreline) offshore.

The analysis of the stratigraphic organization and facies belt arrangement of the delta (see previous Section sedimentary facies belt and sequence stratigraphic subdivision) constituted the basis for the geological model.

A software platform developed by the Hydrogeology Group (GHC; UPC-CSIC) (Velasco *et al.*, 2012b) was used for these tasks. This software was developed in the ArcMap software package and contains a set of tools that enables us to interpret borehole information, create geospatial profiles and to construct a 3D geological model.

Seven stratigraphic surfaces were identified in the boreholes in order to establish the stratigraphic framework. Four of them were derived from the sequence stratigraphic subdivision (i.e. the two sequence boundaries, and the transgressive surface and the maximum flooding surface of the Holocene sequence) and are identifiable by abrupt facies contrasts (Fig. 5.5). Three additional surfaces were defined to constrain the geometry of the significant and correlatable lithostratigraphic units. These were as follows: the top of the discontinuous basal Pleistocene fluvial channel-fill, the base of the regressive delta front in the Holocene regressive systems tract, which separates delta front sands from clays and silts of the prodelta and the limit between fine-grained delta plain deposits and coarse-grained sediments made up of sands and gravels from the delta front and the fill of the main channels in the delta plain of the upper sequence (Fig. 5.5). These surfaces were correlated between the boreholes in the emerged part of the delta, and thirteen cross-sections were generated (see Fig. 5.7). The result of this subdivision enabled us to differentiate between seven units (A to F; Figs. 5.4, 5.5, 5.6, 5.7), which are of sequential significance. The interpolation of the mapped traces from the thirteen cross-sections in non-sampled areas allowed us to obtain a three-dimensional reconstruction of the Besòs delta (Fig. 5.8). The main features of the units distinguished in this model (i.e. lithology and depositional environment) are summarized in Table 5.1 and their extent in the emerged Delta Complex is represented in Figure 5.9.

After the construction of a geological model onshore, an extension of this model offshore was needed to obtain an overall understanding of the delta (see Figs. 5. 6, 5. 10).

From the sequence stratigraphic-based correlation between the onshore-offshore delta (see sequence stratigraphic subdivision), a stratigraphic correlation was also performed owing to the fact that different sequences and system tracts do not develop constant lithological properties.

The progradational delta-front sand-wedge (unit E) at the Holocene RST pinches out approximately 500m from the coastline (after Liquete *et al.*, 2007).

The prodelta muds (Unit D) belonging to the Holocene RST, thin out progressively seawards and cover most of the modelled submerged delta.

The transgressive fan delta front wedge on the TST (Unit C2) thins out seawards. It is not easy to determine its extension on the submarine delta but, the merging of the Postglacial transgressive surface with a transgressive ravinement surface (Gámez, 2007) supports the idea that some sands and gravels extend above the Transgressive Surface several kilometres offshore.

The channel fill gravels on top of the basal boundary of the Postglacial sequence (Unit C1) are difficult to follow offshore since no major channelled erosive surfaces have been distinguished in profile 108 after Gámez (2007) (see Fig. 5.6A, 5.6B). Time-equivalent units corresponding to these channel-fill gravels in the offshore present wedge-shape geometry and depict seaward prograding clinoforms. Probably there was a progradational delta front building (offshore) simultaneously to the channel infill in more proximal areas (onshore).

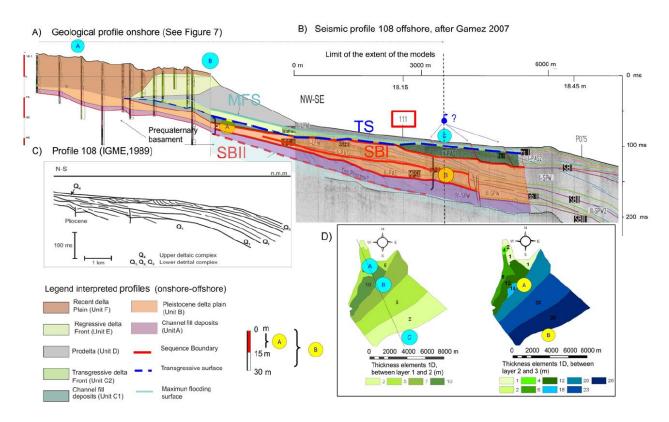


Figure 5.6. A) and B) Correlation of a geological profile onshore A) (for further details and location of this geological profile, see Fig. 5.7) and the interpretation of the seismic profile number 108 of the submerged delta of Besòs after Gámez (2007); B) see location in Figure 5.3. The sequence stratigraphic surfaces and the different units defined can be visualized onshore in the geological profile interpreted (A) and offshore in the interpreted seismic profile. Notice that there is a vertical scale to show the thickness of the units. See also the profile 111 in Figure 5.10 (see location in seismic profile and in Fig. 5.3) and Figure 5.7 and sections: Facies and sequence stratigraphic analysis and Geological model. C) Interpretation of the seismic profile 108 from IGME, (Medialdea et al., 1989). The Upper deltaic complex, unit Q4, correlate with the regressive and the transgressive systems tract of the Postglacial sequence described; the lower detrital complex comprises the units Q3, Q2 and Q1, and correlates with Postglacial late lowstand systems tract, and with the Pleistocene sequence described herein. See Figures 5.5 and 5.7 and section Facies and sequence stratigraphic analysis for more details. D) Thickness maps of the aquitard's elements of the hydrogeological model. Notice that also these maps show the location of the profile onshore-offshore exposed in A and

Nevertheless, this Unit is easily identified above the upper sequence boundary (SBI) in the profile 111 (see Fig. 5.10).

Delta plain muds in the Pleistocene unit B were difficult to identify in the offshore domains since most of the reflectors show clinoform geometries related to coastal and submarine progradation. Thus, these delta plain sediments (unit B) quickly pass offshore to coastal and marine facies.

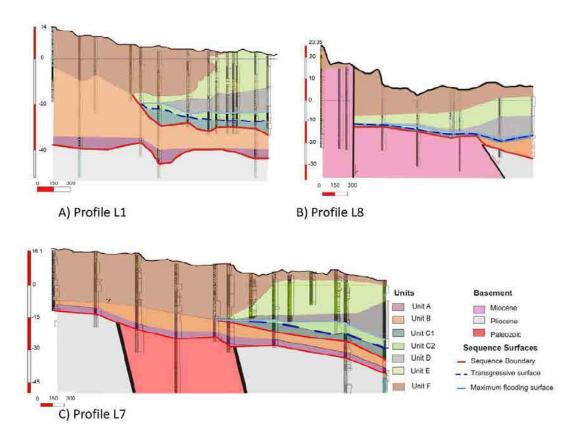


Figure 5.7. Three cross section perpendicular to the coast. The sequence stratigraphic surfaces and the different units can be visualized. The location is showed in Figure 5.8A. See section geological model for detailed description of the units and the sequence stratigraphic interpretation.

Channel fill gravels (Unit A) are associated with the lowermost sequence boundary (SBII) and are not easy to correlate offshore from the seismic data interpreted by Gámez (2007) in the seismic profile 108. This surface is probably a surface where other sequence boundaries coalesce. Figure 5.9 shows that Unit A infills NW-SE oriented paleovalleys onshore. This was born in mind when including the NW-SE elongated gravel units corresponding to Unit A in our offshore model.

As shown in Figure 5.6B, a series of normal faults (some of them lystric) were observed at a distance of 5km offshore. At this point, Unit D reaches its minimum thickness and is cut by these faults, which lead us to strongly consider a connection of the main aquifer units (constituted by C1 and C2) with the Sea.

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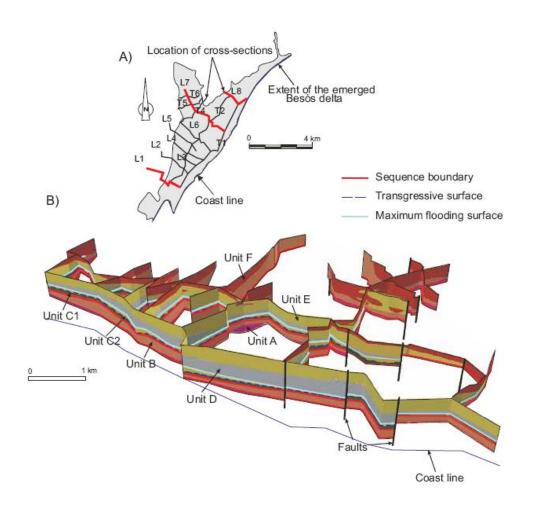


Figure 5.8. Location of the cross section performed to construct this fence-diagram (notice that the location of the cross section of the Figure 5.7 are coloured in red), B) Geological model of the Besòs delta viewed by means of thirteen cross-sections generated, showing the geometry and continuity of the seven geological units distinguished (view is from E). This model has been performed by using a software platform developed by the Hydrogeology Group (GHS; CSIC-UPC) (for further information see Velasco et al., 2012b). The sequence stratigraphic surfaces (i.e. sequence boundaries, the transgressive surface and the maximum flooding) are also indicated. See characteristics (i.e. lithology, depositional environment and hydraulic behaviour) of the geological units distinguished in Table 5.1.

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Deltaic depositional environment	Facies association	Description	Geometry	Geological units of the model
Delta plain	Fluvial channel	Poorly sorted gravels, occasionally with sandy matrix and some lenses of organic matter. The pebbles are well rounded and polymictic	Concave up-shape	$\boldsymbol{A}$ , C1, and part of B and F
	Floodplain	Red and yellow clays	Large extension and lateral continuity	F, B ( part of)
	Alluvial fan	Interbeded deposits of heterometric gravels and sands derived from sourronding relieve	Sheet-like shape	F, B (part of)
Delta front	Regresive Delta front	Yellow to gray coarse grained facies belt made up by sands and gravels. (from distal to proximal). Shells fragments	Dipping clinoform shape and flat bases	E
	Transgresive delta front	Gravels well rounded to angular pebbles with sand. Sparse shell fragments	Large extension and lateral continuity	C2
Prodelta	Prodelta	Grey clay and silts with intercalation of fine sand and with marine fauna	Wedge shape	D

Table 5.1. Facies association, description, geometry and correlation with the different units defined for the geological model of the depositional environments distinguished in the Besòs Delta.

# 5.4.2 The hydrogeological model

# 5.4.2.1 Definition of the aquifers and the status of groundwater

A number of specific issues must be considered when dealing with groundwater in extensive urbanized areas such as the Besòs delta. Urbanization has a major impact on the quality and quantity of groundwater resources. The main difference between groundwater analysis in urbanized areas and groundwater analysis in natural systems lies in the evaluation of recharge since different water sources are involved in urbanized areas. In addition, groundwater can affect subsurface city infrastructures such as public transport services and conductions (Vázquez-Suñé et al., 2005).

Traditionally, the aquifers of the Besòs delta were mainly exploited for industrial and domestic purposes. Until 1940, their exploitation was moderate, and was mainly concerned with watering and domestic supply. Subsequently, water extraction increased until it reached 66hm<sup>3</sup>/yr in the late 1960s because of the growth of industrial activity (MOP, 1966; Ondiviela *et al.*, 2005). This extraction led to overexploitation of the aquifers of the area, bringing about a marked decrease in the phreatic level, which resulted in marine intrusion (Vázquez-Suñé and Sánchez-Vila, 1999). In order to mitigate the progressive salinization of the aquifers, the possibility of recharging them with treated residual water has been considered (Custodio et al., 1976). Deterioration of the quality and quantity of water from the aquifer due to its overexploitation and due to dumping waste into the river and subsoil obliged many industries to discontinue groundwater extraction or to move outside the urban area. Since the1960s, the extraction in the Besòs delta aquifers has decreased, with an estimated figure of 20hm<sup>3</sup>/yr. The reduction in extraction involved the recovery of the aquifers, which increased infiltrations in many underground infrastructures (Ondiviela *et al.*, 2005). At present, the Catalan Water Agency (*i.e.* ACA, Agència Catalana de l'Aigua) is developing a groundwater management

programme to recover groundwater quality and quantity with the aim of guaranteeing sustainable pumping rates.

The hydrogeological model presented in this paper involved an exhaustive review of previous hydrogeological works developed in this area (e.g. Moragas, 1896; Rubio and Kinderlán, 1909; MOP, 1966; Nilsson et al., 2002; Ondiviela et al., 2005; Ferrer, 2005; Tubau et al., 2009; De Buen, 2009). The proposed model makes use of the geological characterization of the Besòs delta and the subsequent geological model. As a result, three aquifer units and two aquitards in the Besòs delta were identified and their geometry and connection were characterized by the 3D geological model (see the geological model section and Table 5.2).

#### I. AQUIFER UNITS:

#### a. Lower aquifer:

It is mainly constituted by a Pleistocene fluvial channel (Unit A). These deposits rest unconformably on the top of relatively impermeable Paleozoic to Cenozoic rocks and deepen seawards. Moreover, in some parts of the Delta Complex, the fluvial channel deposits and the alluvial fan of the Pleistocene Delta Plain (Unit B) increase the thickness of this aquifer.

# b. Main aquifer:

This comprises units C1 and C2 and is the main aquifer of the Besòs delta. Unit C1 is constituted by a fluvial channel and unit C2 corresponds to the aforementioned transgressive delta front facies association.

#### c. Shallower aquifer:

A third, shallower aquifer corresponds to unit E, which is formed by the Holocene regressive delta front. In addition, the coarser deposits of Unit F (alluvial fans and fluvial channels) partially cover Unit E, thickening the shallower aquifer.

#### II. AQUITARD UNITS:

# a. Lower Aquitard:

The main aquifer is separated from the lower aquifer by a less permeable body corresponding to unit B, which is constituted by Pleistocene delta plain sediments.

#### b. Upper aquitard:

The shallower aquifer is separated from the main aquifer by the Holocene prodeltaic unit D, which is less permeable. Unit D peters out landwards, allowing a partial connection between the shallow and the main aquifers. In addition to defining the aquifer and aquitard

units, the conceptual hydrogeological model of the Besòs delta necessitated the determination of other input variables, such as areal recharge or groundwater extractions. In the Besòs delta, the areal recharge was estimated taking into consideration the sewage system and loss in water supply (Vázquez-Suñé et al., 2005). Besides, groundwater extractions have been evaluated taking into account information from industries and water supply wells.

# 5.4.2.2 Hydrogeological modeling

A quasi-3D model was built to simulate groundwater flow and chloride transport in the Besòs Delta aquifers. The flow and transport problem used a finite element grid of 2977 nodes and 6565 elements divided into three layers. The top layer represents the shallower aquifer, the intermediate layer the main aquifer, and the bottom layer represents the lower aquifer. In order to establish the connection between the aquifer layers, one-dimensional elements were defined between each layer. These one-dimensional elements represent the layers defined in the geological model as less permeable units D and B, and were assigned their corresponding thicknesses. The submerged portion was modeled by extending the model domain 5km seawards (Fig. 5.6, 5.8).

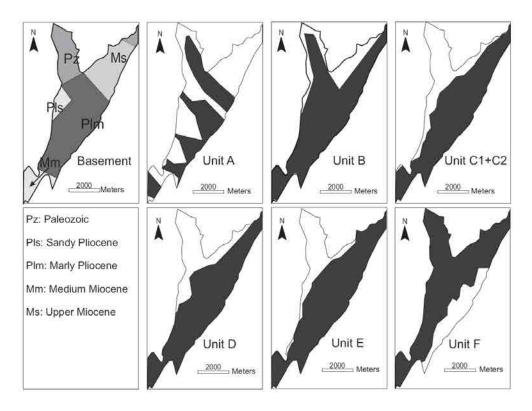


Figure 5.9. Map showing the spatial distribution of the different units considered and of the basement.

[Chapter 5: A sequence stratiraphic based geological model for constraining a hydrogeological model in the Besòs Delta (NW Mediterranean coast, Spain)]

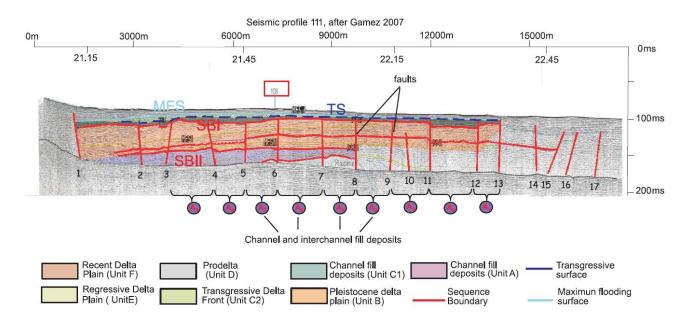


Figure 5.10. Interpretation of the seismic profile 111 (after Gámez 2007). See Figure 3 for location. The sequence stratigraphic surfaces, the different units and the set of faults that conditioned the orientation of the interpreted interchannels and channels deposits (numbered from A1 to A9) can be visualized. As well, the interpreted interchannels and channels can be visualized in Figure 5.11.

Age	Geological units	Sedimentary environmental deposits/ Facies association	Hydrogeological units	Description Hydrogeological units
Post-glacial	F	Delta Plain (floodplain deposits)		Less permeable unit
	F	Delta Plain( fluvial channel fill deposits and alluvial deposits) Regressive Delta Front	_ Layer 1	Shallower aquifer
	D	Prodelta	One-dimensional layer 1	Less permeable /aquitard
	C2	Transgressive Delta Front		Main Aquifer
	C1	Fluvial Channel fill deposits (Delta plain)	Layer 2	
Pleistocene	В	Delta Plain(floodplain deposits)	One-dimensional layer 2	Less permeable /aquitard
	В	Delta Plain (fluvial channel fill deposits)	Layer 3	Lower Aquifer
Pe	Α	Fluvial channel deposits		

Table 5.2. Geological units, facies association, hydraulic behaviour and correlation with the different units defined in the hydrogeological model of the Besòs delta.

Variable density effects were not considered in the numerical model given that vertical fluxes can be neglected in aquifers with small thicknesses, as in the case of the Besòs Delta aquifers (Abarca *et al.*, 2006). Equally, lateral variable density fluxes were also neglected in the model since their effect is considerable when the lateral slope exceeds 3% (Abarca *et al.*,

2007), which is not the case in the Besòs delta. By contrast, the significant effect of boundary heads was integrated into the model by defining seaside boundary conditions in terms of equivalent freshwater heads.

Visual Transin (GHS, 2013d) is a graphical user-friendly interface for TRANSIN (Medina and Carrera, 2003; Medina et al., 2000), which allows simulation and calibration of flow and transport parameters. This code was used for automatically calibrating the numerical model versus both head and chloride data. Three conditions must be met when calibrating the model: consistency between prior information and calibrated values; a good fit between measured and computed data in terms of both piezometric heads and chloride concentrations; and consistency between water and chloride mass balances with respect to the conceptual model and previous calculations. In the hydrogeological model of the Besòs delta, spatial discretization is refined near the main pumping areas, and the mesh is adapted to the main hydrogeological features. The average size per element is about 100m in length. The model was calibrated by using historical data of water management and production in the last hundred years. Calibration time was set from 1915 to 2006 inclusive. The calibration procedure necessitated the prior estimation of all the model parameters, which were mainly based on data integration and geological review. For instance, 46 transmissivity zones were initially defined. The definition of these zones were conditioned to: the geometry and thickness of the different sedimentological bodies, the textural properties of each defined facies correlated with permeability values, and finally the punctual values obtained from hydraulic testing (performed for this study and derived from previous studies).

In general terms, the transmissivity values obtained by calibration satisfactorily fitted the information provided by the conceptual model. Figure 5.11 shows the transmissivity values calibrated for the model. Transmissivity tends to be higher in the areas of the aquifer where the grain size is coarser, and especially where the fluvial channels are presumably located.

[Chapter 5: A sequence stratiraphic based geological model for constraining a hydrogeological model in the Besòs Delta (NW Mediterranean coast , Spain)]

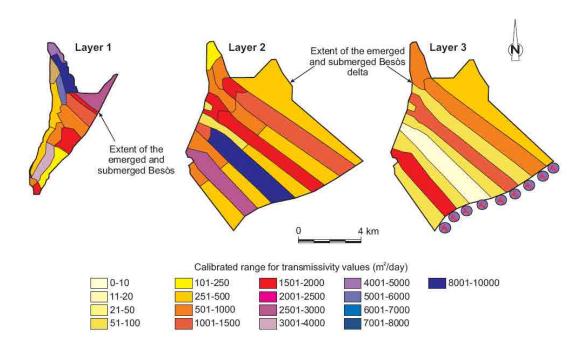


Figure 5.11. Maps showing the transmissivity values obtained by calibration for the aquifer layers. Layer 1 corresponds to the shallower aquifer; layer 2 corresponds to the main aquifer; and layer 3 is the lower aquifer (see Table 5.2).

A similar procedure of calibration was used with the remaining parameters (*i.e.* storage coefficient, areal recharge, boundary flows, and pumping rates), obtaining a satisfactory fit both in terms of heads and chloride concentrations. The calibrated model yields a reasonable fit between measured and calculated data for both chloride concentration and head (Fig. 5.12).

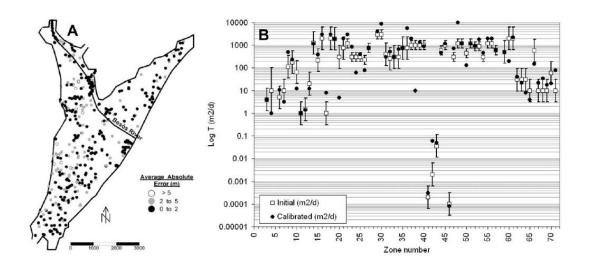


Figure 5.12. A) Map of average error rate. Error values are indicated in meters. B) Graph showing the previous transmissivity values versus the final calculated values. The vertical bars represent the assumed standard deviation for previous transmissivity values.

# 5.5 Discussion

# 5.5.1 The role of sequence stratigraphy in geological and hydrogeological modeling

The geological model of the Besòs delta was developed using a sequence stratigraphic approach. Sequence stratigraphy has been used in the oil industry for decades (*e.g.* Mitchum, 1977; Payton, 1977; Vail *et al.*, 1977; Posamentier and Vail, 1988; Van Wagoner *et al.*, 1990). This approach offers an interesting perspective on the architecture of sedimentary bodies when geological controls and processes are considered.

A number of modeling studies have highlighted the importance of a sequence stratigraphic analysis when modeling reservoir heterogeneity. Ainsworth *et al.*, (1999) compared flow responses from models that used a lithostratigraphic correlation and those that employed chronostratigraphic correlation in a lacustrine delta in the Sirikit field (Thailand). The studies of Cook *et al.* (1999) and Larue and Legarre (2004) focused on a shallow marine reservoir in the Meren field (offshore Nigeria). In the former work, a sequence stratigraphic analysis was used to determine the geological framework of marine flooding surfaces and sequence boundaries on which the facies modeling was based. These authors concluded that the vertical compartmentalization in the reservoir was mainly produced at the flooding surface which separated mudstone beds from sandstone deposits. The study of Larue and Legarre (2004) revealed the differences in trapped oil distribution predicted by models based on a detailed sequence stratigraphic analysis and those based on a large scale analysis. A

very detailed sequence stratigraphic subdivision of a transgressive-regressive sequence of an outcropping fan-delta was used by Cabello *et al.* (2010) and Cabello *et al.* (2011) as a modeling framework to reproduce the interfingering scales that controlled distribution of facies associations that may affect flow.

Owing to the parallels between sedimentary reservoirs and aquifers, the present paper makes use of sequence stratigraphy to provide new insights into the Besòs delta architecture and to derive geological and hydrogeological models. This methodology is in line with several studies of aquifers such as those by Sugarmann and Miller (1996); Pendas (2002); Houston (2004); Gámez (2007); Gámez et al. (2009) and Scharling et al. (2009).

There were three reasons for adopting the sequence stratigraphic approach in the Besòs delta:

Given the variety of the dataset and given the complexity and variability of facies distribution in the delta, the identification of the surfaces using sequence stratigraphy yielded a good correlation between the boreholes for the emerged part of the delta. The sequence stratigraphic subdivision was undertaken by: the identification of different depositional environments, the identification of progradational-retrogradational and coarsening or fining upwards trends and the detection of sharp erosive surfaces.

The characterization of the submerged part of the delta was not easy, given the lack of onshore-offshore geological mapping. In this regard, the methodology of sequence stratigraphic correlation offers an optimum approach since it is able to provide tools to correlate interpreted surfaces and system tracks onshore and offshore. We undertook a sequence stratigraphic correlation between the emerged delta and 5km of the submerged delta, which enabled us to obtain an overall framework for the quaternary architecture of the Besòs delta.

The sequence stratigraphic surface correlation allowed us to constrain the distribution of facies associations more reliably than using lithostratigraphic-based correlation and modeling. The resulting subdivision into seven geological units by means of sequence stratigraphic and subordinated lithostratigraphic surfaces satisfactorily represents the petrophysical properties found. This provides a more realistic assignment of the hydraulic properties for each geological body.

The deltaic nature of the stratigraphic succession enabled us to apply the sequence stratigraphic approach to this study because coastal and deltaic depositional systems record relative base-level changes. By contrast, in continental environments, the difficulty of identifying key surfaces (*i.e.* sequence boundaries, transgressive or maximum flooding surfaces) rules out sequence stratigraphic analysis. In coastal and deltaic systems, the delta front, which is made up of coarse-grained deposits arranged in continuous and extensive bodies, constitutes the main aquifer unit, as in the Besòs delta. This facies association is most

sensitive to relative base-level fluctuations and, as a result, sequence stratigraphic analysis is necessary to characterize aquifers in this type of depositional systems.

# 5.5.2 The geological model

In the emerged part of the Besòs delta, an average of about 22 boreholes per km<sup>2</sup> was available. In this very densely sampled scenario, a deterministic reconstruction of the defined geological units was considered as the best approach to interpret the most relevant sedimentological heterogeneities in the delta for a regional scale. Although more detail can be captured when modeling sedimentary heterogeneity at the scale of facies distribution, the design of the hydrogeological model in the Besòs delta introduced an accurate discretization of the hydraulic properties taking into account the internal heterogeneity of the geological units defined, *i.e.* facies distribution within facies associations.

Nevertheless, despite widespread sampling in the Besòs delta and despite the application of sequence stratigraphy, the nature and variability of proximal-to-transitional facies in the regressive systems tract of the Postglacial sequence introduced some uncertainty into the correlation process. In this zone, fine sediments frequently alternate with coarse-grained deposits, which made it difficult to differentiate between coarse sediments of the delta plain (channel fill deposits) and those of the delta front. In addition, the alluvial wedges, which are derived from the surrounding reliefs and are locally connected to the delta front body, make the delimitation of the stratigraphic units more uncertain. Moreover, the identification of the limit between the Pleistocene and the Postglacial sequences in the proximal deposits of the delta plain was prevented by the absence of sedimentary surface expressions. By contrast, characteristic lithologies and sequence stratigraphic significance were clearly defined in the marine deposits of the delta.

In outcropping depositional systems, correlation in continental environments can be carried out more effectively because of the availability of geological data (López-Blanco, 1996; López-Blanco *et al.*, 2000a, b), which enabled us to improve the 2D and 3D modeling of the heterogeneous media (Cabello, 2010).

As for the onshore-offshore correlation, large uncertainties should also be taken into account for the positioning of some surfaces and systems tracts owing to the scarcity and nature of the offshore data. One example of this is the identification of the lower sequence boundary defined onshore (SBII), which is probably a surface where other sequence boundaries coalesce offshore.

Another related uncertainty is the distribution of the geological units, within the offshore part of the model, that were defined by our conceptual understanding of the system and the offshore-onshore correlation of system tracts and surfaces.

# 5.5.3 Applicability of the workflow modeling

Although several groundwater flow and transport models have already been developed for the main and the upper aquifers in the Besòs delta (Vázquez-Suñé and Sánchez-Vila, 1999; Ondiviela, 2003; Vázquez-Suñé et al., 2005; Ferrer, 2005; Tubau et al., 2009; De Buen, 2009), these models did not take into account the lower aquifer or its interaction with the whole system. The hydrogeological model of the Besòs delta presented in this paper is a considerable improvement on the aforementioned contributions because of a better geological characterization and the incorporation of the lower aquifer. Moreover, given that the calibration of the hydrogeological model resulted in a robust solution with recalculated hydraulic values that were consistent with the geology of the delta, it may be assumed that the hydrogeological model validates the geological model. An unrealistic geological model as a basis for hydrogeological modeling would hamper the calibration of the hydraulic properties.

# 5.6 Conclusions

The application of sequence stratigraphy enabled us to develop a consistent 3D geological model of the basin, which provides valuable insights into the distribution of hydraulic parameters.

As a result of the significant improvement in the characterization of the geological heterogeneity of the Besòs Delta Complex, the lower aquifer was incorporated into the model, which further improves our understanding of the hydrogeological characteristics of the Delta.

The consistency of the hydrogeological model validated the geological model and demonstrates the definite advantages of the methodology used in our study .This workflow modeling can be used to design and optimize hydrogeological modeling in similar settings, especially in urbanized areas where an effective management of groundwater is essential because of the subsurface infrastructures and the high population density.

Finally, the modeling platform used enabled us to structure all the available data and to set up an updatable model database, which makes this model ideal for future updates and downscaling.

# **6 GENERAL CONCLUSIONS**

This chapter provides a summary of the main findings of this thesis.

The first contribution of this research is the development of a GIS-based software platform that arranges all the available hydrogeological data into a coherent structure and provides support for its proper management, analysis, interpretation, pre and post-processing for modelling.

One of the main components of this software platform is the geospatial database HYDOR (chapter 2), which represents geospatial information based on the *Personal Geodatabase* structure provided by the ArcGIS (ESRI) concept. In line with this approach, a number of advantages should be highlighted. First, the structure of the spatial database allows us to store data for the majority of geological and hydrogeological studies. This type of database has bee designed to manipulate spatial and time-dependent information more efficiently than other platforms and allows the user to store and manage detailed hydrogeological information that can be subsequently upscaled and updated. In addition, the possibility of querying and visualising the stored information allows the user to integrate all the data and thus obtain further relevant information. The integration of detailed core stratigraphic and lithological descriptions with local and regional hydrogeological parameters, hydrochemical analyses, hydrogeological tests (pumping and tracer), hydrologic, geophysical and geotechnical information, etc provides the user with a consistent image of the behaviour of the aquifer under study.

Another important advantage is that the use of the spatial database facilitates data integration concerning land-use, infrastructure design, and environmental aspects. The relationship between the groundwater and the main urban contaminant factors (sewerage system, water supply network, etc.) and the interaction of the groundwater with major civil works (subway tunnels, underground parking lots, etc.) is highlighted. As a result, it is possible to study different problems in a more realistic manner to improve our understanding of the geology and hydrogeology of urban areas.

The introduction of data is facilitated by alternative utilities such as intermediate tables, inherent GIS wizards and assisting menus following a pre-established entry protocol.

Despite the large amount of data that can be stored, their consultation is simple by using the GIS-tools developed which enable the visualisation and analysis of hydrogeological data. These instruments were developed as an extension of the ArcGIS environment and have the form of three toolbars integrated into ArcMap.

The first set of tools regrouped in the HEROS toolbar (chapter 3) allows us to perform a detailed geological analysis and the 3D representation of the interpreted geological

features. One of these tools enables us to obtain stratigraphic columns, where information such as texture, lithology, fossil content, chronology, results of insitu tests and earlier interpretations is shown together. This is an optimum environment for facilitating the interpretation and the identification of different sedimentary units/subunits. The software platform also contains tools that support a variety of workflows for creating cross sections. This system allows the modelling of the distribution and geometry of the sedimentary bodies by knowledge-based control of the modeller. As shown in this thesis, the 2D features defined in the cross sections can be converted into a 3D environment. The resulting 3D features can be visualised as fence-diagrams in the same GIS environment using ArcScene or can be exported to external software packages to construct the 3D geological model. The design of the tools presented is in line with the classic working instruments used by geologists to characterise a study area.

The second toolbar (QUIMET, chapter 4) was specifically designed for performing graphical and statistical analyses of hydrochemical parameters. For instance, the Statistical Quimet Tools offer the user a comprehensive statistical analysis of data including descriptive statistical analysis, bivariate analysis, generation of correlation matrix and correlation graphics, etc. Furthermore, the multi-choice query forms belonging to the Spatial Analysis Tools provide multiple queries for comparing temporally and spatially groundwater parameters. Moreover, useful calculations of hydrochemical parameters (e.g. ECB, ionic ratios, etc), thematic maps, and plots with temporal evolution of parameters or pre select data for further geostistical analyses, etc can be easily obtained.

The last toolbar, termed HYYH (chapter2), comprises utilities for a reliable analysis of hydrogeological data and hydraulic experimental data. Contour maps and further spatial operations representing the depth or thickness of the hydrogeological units (e.g. aquifers, aquitards, etc) could be generated using customized queries. Likewise, piezometric maps can be created for the selected points and for the selected period of time with another command included in this toolbar. Another command consists in multi-criteria query forms that allow us to analyse different data and interpretations derived from pumping and tracer tests (such as transmissivity, storativity, permeability), and to represent them in a map as point features.

The interpreted data and calculations by using the aforementioned tools can be easily stored and consulted in the same platform and can be used to build an updatable model database for subsequent interpretations. Thus, each model study does not have to start from scratch.

These tools were implemented in the same ArcGIS software package and their analysis potential was extended taking advantage of the additional inbuilt instruments of this platform (e.g. Geostatistical tools, Analysis tools). Furthermore, ArcGIS fosters a shallow learning curve, the easy maintenance and the interoperability among different tools owing to its widespread adoption.

Moreover, this software platform offers interoperability with external software for subsequent analyses of hydrogeological data, such as hydrochemical modelling packages like MIX code.

Another major contribution of this thesis consists in the generation of a comprehensive working framework of groundwater resources for the metropolitan area of Barcelona (NE, Spain). This has been made possible by the implementation of the database model HYDOR for this area together with the use of the aforementioned GIS-tools.

In chapter 5, a detailed hydrogeological model of the Besòs Delta (located in the metropolitan area of Barcelona) is offered as an example of applicability of the software platform proposed. The integration of the available data into the HYDOR geodatabase and the use of the GIS-tools allowed us to 1) delimit the geological units by means of sequence stratigraphic subdivision, 2) generate the 3D facies belt-based model of the Besòs Delta built on the basis of this geological characterisation and 3) use this model to constrain the distribution of hydraulic parameters and thus obtain a consistent hydrogeological model of the delta, which was calibrated by water management and production data recorded over the last hundreds years. Because of this marked improvement in the characterisation of the geology of the Besòs Delta complex, the lower aquifer was incorporated into the model, which significantly contributes to our understanding of the hydrogeological characteristics of the delta.

Other examples of applicability of this platform software are showed in chapter 2, 3 and 4. Apart from these projects performed in the urban area of Barcelona, this platform has been successfully used in several projects such as, Geo3D, 2010; UPF, 2011; Matraz-UPC, 2012 and AMB, 2013.

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#### ANNEX 1: ARTICLES AND REPORTS RELATED TO THE DEVELOPMENT OF THIS THESIS

#### **Annex 1.1. Scientific Articles**

- Velasco, V., Cabello, P., Vázquez-Suñè, E., López-Blanco, M., Ramos, E., & Tubau, I. (2012). A sequence stratigraphic based geological model for constraining hydrogeological modeling in the urbanized area of the Quaternary Besòs delta ( NW Mediterranean coast , Spain ). Geologica Acta, 10, 373–394. doi:10.1344/105.000001757.
- **Velasco, V.**, Gogu, R., Vázquez-Suñè, E., Garriga, a., Ramos, E., Riera, J., & Alcaraz, M. (2012). The use of GIS-based 3D geological tools to improve hydrogeological models of sedimentary media in an urban environment. Environmental Earth Sciences. doi:10.1007/s12665-012-1898-2.
- **Velasco, V.**, Tubau, I., Vázquez-Suñè, E., Gogu, R., Gaitanaru, D., Alcaraz, M., Serrano-Juan, A., Fernàndez-Garcia, D., Garrido, T., Fraile, J., Sanchez-Vila, X (2013, Submitted and accepted with revisions). GIS-based hydrogeochemical analysis tools (QUIMET). Computers & Geosciences.
- **Velasco, V.**, Criollo, R., Vázquez-Suñè, E., Alcaraz, M., Serrano, A., García-Gil, A., Gogu, R. GIS-based Hydrogeological database and analysis tools, (2013, submitted). Environmental Modelling & Software.
- R. Gogu, **V. Velasco**, E. Vazquez, D. Gaitanaru, Z. Chitu, I. Bica, (2011). Sedimentary media analysis platform for groundwater modeling in urban areas. Advances in the Research of Aquatic Environment, Vol 2, Springer Verlag, ISBN -978-3-642-24076-8, DOI 10.1007/978-3-642-24076-8.
- Gogu.R, **Velasco.V**, Garriga.A, Monfort.D, Vázquez-Suñe.E, Carrera.J, Ramos.E, (2010), "Platformă Informatică pentru integrarea informației pentru medii sedimentare în vederea obținerii unui model hidrogeologic 3D", ROMAQUA, Ed. Asociația Română a apei, pp. 22-31, Volumul 2, 2010, ISSN 1453-6986, București, România.
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- Bellmunt.F, Marcuello.A, Ledo.J, Queralt.P Falgàs.E, Benjumea.B, **Velasco. V**, Vázquez-Suñé.E (2012). Time-lapse cross-hole electrical resistivity tomography monitoring effects in an urban Tunnel. Applied Geophysics, Vol 87, 60-70.

### **Annex 1.2. Proceedings**

- Velasco, V., Vázquez-Suñè, E., Criollo, R., Alcaraz, M., Serrano-Juan, A., García-Gil, A., Tubau, I., Gogu, R., Gaitanaru, D., (2013, submitted and accepted under revisions). GIS-based Hydrogeological Database and Analysis Tools. INFOCOMP2013. The Third International Conference on Advanced Communications and Computation. 17-22 Noviembre, Lisboa (Portugal).
- Velasco.V, Tubau.I, Vázquez-Suñè.E, Gaitanaru.D, Gogu.R, Alcaraz.M, Serrano.A, Sánchez.X, Fernandez. D, Fraile.J, Garrido.T (2012). GIS based Hydrochemical Analysis Tools (QUIMET). 7th EUREGEO, Bolonia, Italia, Junio 2012. Vol1, 419-420.
- Gogu .R, Gaitanaru.D, Chitu.I, Ionita.A, Palcu.M, Velasco.V, Vazquez-Suñe.E, Batali, Bica.I (2011). Sedimentary Media Modelling Platform for Groundwater Management in Urban Areas.EGU, General Assembly 2011. Geophysical Research Abstracts, Vol. 13, EGU2011-12498.
- Velasco.V, Cabello.P, Vázquez-Suñè.E, López-Blanco.M, Ramos.E, Tubau.I (2011) Un modelo geológico basado en estratigrafía secuencial para realizar un modelo hidrogeológico del área urbana del delta del Besòs (NW de la costa mediterránea, España).Congreso Ibérico sobre las aguas subterráneas: Desafíos de la gestión para el siglo XXI., Zaragoza, 2011.
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- Velasco. V, Garriga. A, Gogu.R, Monfort.D, Vazquez-Suñé.E, Carrera.J Ramos.E (2008).

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## ATENCIÓ i

Les pàgines 157 a 206 de la tesi contenen els articles citats a l'annex 1.1, que es poden consultar a la web dels diferents editors.

# ATENCIÓN i

Las páginas 157 a 206 de la tesis contienen los artículos citados en el anexo 1.1 de la tesis, que pueden consultarse en el web de los diferentes editores.

## ATTENTION i

Pages 175 to 206 of the thesis, Annex 1.1. Scientific Articles, are availables at the editor's web