3D Modelling and Geothermal Potential Assessment of a Fractured Carbonate Reservoir in the South-Eastern Pyrenees. The Empordà Case Study in NE Catalonia - GeoERA HotLime Project

Ignasi Herms^{a*}, Montse Colomer^a, Gerold W. Diepolder^b, Guillem Piris^c, Georgina Arnó^a, Enrique Gómez-Rivas^d, Anna Gabas^a, Irene Cantarero^d, Fabiant Bellumnt^a, Anna Travé^d, Albert Macau^a, Albert Griera^b, Beatriz Benjumea^a, José Sedano^a, Sara Figueras^a, Juan Diego Martín-Martin^d, Telm Bover-Arnal^d, David Healy^d

^a Institut Cartogràfic i Geològic de Catalunya (ICGC), Parc Montjuïc E-08038, Barcelona, Spain

^b Bavarian Environment Agency (LfU) – Geological Survey, Bgm.-Ulrich-Str. 160, 86179 Augsburg, Germany

^c Departament de Geologia. Universitat Autònoma de Barcelona (UAB) 08193 Cerdanyola del Vallès, Barcelona, Spain

^d Facultat de Ciències de la Terra, Universitat de Barcelona (UB), Martí i Franqués, s/n, 08028 Barcelona, Spain

(*) ignasi.herms@icgc.cat

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ABSTRACT

This paper presents the preliminary results of the characterization of the low enthalpy geothermal resource in the lower Tertiary fractured limestone aquifer within the Empordà Basin, located in the north-eastern sector of the untrusted foreland basin of the Pyrenees in NE Catalonia. The case study is included in the GeoERA HotLime project (co-financing H2020), which addresses the mapping and assessment of geothermal plays in deep carbonate rocks from different pilot areas in Europe. A new 3D geological and thermal model of the reservoir-bedrock system has been developed through an integrated interpretation of the previous geological, geophysical and geothermal information available in the study area, complementing it with new geophysical and rock sampling campaigns. The overall available information has been used to develop a 3D conductive layered based steady state regional heat flow model applying a heat uncertainty analysis, to infer the probable temperature distribution within the basin. The geothermal potential assessment has been addressed using the new 3DHIP-Calculator tool, a Matlab-based software compiled for windows which allows to stochastically apply the Heat-In-Place method (Muffler and Cataldi, 1978, Muffler, L.J.P., 1979) by using 3D voxel models. Then by means of geographical information system, the georeferenced output results have been converted in raster maps showing among them the spatially distributed stored heat energy (PJ/km²) under different probability scenarios (P10%, P50% and P90%). These maps allow to identify the most favourable and promising areas to go forward for the planning and development of new prospections at local scale.

1. INTRODUCTION

Deep carbonate geothermal reservoir has been of interest in Europe (EU) as they contain low-to-medium temperature fluid reservoirs useful for direct uses and many times for CHP generation. The most well-known examples of tapped resources in EU are in Paris Basin (France) and Molasse basin (Germany) which exploit resources located within Mesozoic deep aquifers since many years ago. Spain also have potential for low-to-medium resources (Arrizabalaga, I., 2020). In Catalonia (NE, Spain) the most favourable areas are localized mainly in the Ebro River basin and the Neogene basins related to the Catalan Coastal Ranges (such as the Vallès basin, Reus Valls Basin, Empordà, La Selva, etc). These geothermal resources, if deployed and harnessed adequately through new studies and proper development initiatives, could help for instance to decarbonize the heating and cooling sector in different energy high demanded areas. Nevertheless, one of the main troubles to develop projects is the necessary initial investment to prove and characterize the resource. The geological knowledge of the deep major geothermal areas in Catalonia and Spain in general, is far from what is available in other countries like France, Germany or Switzerland, because in the last 30 years, there has been almost no exploration. In fact, deep geological knowledge (>1500m) in terms of reservoir characterization is limited. This is one of the reasons among others likewise important, why geothermal projects have been hampered so far in Spain and consequently in Catalonia too: the lack of information on the hydrogeological characteristics of existing deep aquifers.

The oil and gas industry in the 1960's and 1970's made different studies exploring the subsoil by means of seismic campaigns and with few deep wells in different places around Catalonia. Afterwards some exploration studies were carried out in the 1970's and 1980's by the Instituto Geológico y Minero de España (IGME, 1976, and others later) which includes geophysical works, geochemical sampling and some shallow exploration wells (mainly 200-500m depth). These studies were based on the available formation obtained from old deep hydrocarbon exploration wells did in 1960's which served to identify several Mesozoic and Tertiary permeable formations. The low-enthalpy geothermal play of the Empordà basin located in the north-eastern sector of the untrusted foreland basin of the Pyrenees in NE Catalonia was one of the promising identified areas. In this, it was identified a deep and hot fractured carbonate reservoir in the lower Eocene. This reservoir has been up to now of interest at least two times for different private initiatives: for spirulina production in the 80's and for new hotel-spa project in 2000s (PH, S.A. 2003). However, there is no detailed evaluation at the aquifer scale. The unique available resource assessment at regional scale for the whole territory of Spain was prepared with the framework of the PER 2011-2021 technical study titled 'Evaluation of the geothermal energy potential' (Sánchez-Guzman, et al., 2011). This was based on the available data gathered by (IGME, 1976). The rough assessment of accessible geothermal resource base was did using the well-known volumetric "Heat In Place" (HIP) method proposed by the US Geological Survey (USGS) (Muffler & Cataldi, 1978; Muffler, L.J.P., 1979) following a deterministic approach (fixed values) and a regional unit model (estimation for the entire reservoir).

The HIP estimation is the first and the key step of any geothermal project in early exploration stages. The HIP method its subsequent revisions and new proposals for specific reformulations (Williams, et al., 2008, Garg & Combs, 2011, 2011, 2015) is the evaluation technique for the estimation of the available stored and recoverable heat from deep geothermal reservoirs most globally used today among geological services, research centres and companies in general. The methodology that was originally defined should use the stochastic approach proposed initially by Nathenson (1978) to consider the uncertainty in the accessible geothermal reservoir, the re-injection or reference temperature, and the properties of the water-rock system: porosity, density, and specific heat capacity.

In the simpler form of applying the HIP method, the reservoir is conceptualized as a unit model (one-cell approach) for its entire volume or considering a specific part of it, and therefore the stored heat is estimated as a whole (Arkan & Parlaktuna, 2005; Halcon et al., 2015; Yang et al., 2015, Barkaoui et al., 2017; Shah, et al., 2018; Miranda et al., 2020). This is normally performed using commercial software such @Risk (Palisade) or Cystall-Ball (Oracle). This approach can be also applied nowadays using free and open-source tools (Pocasangre & Fujimitsu, 2018). Altough originally the HIP method was tought to be applied following a stoachstic approach using Monte Carlo simulations, many authors has been also applied it following a determinitic approach at regional scale (Colmenar-Santos et al., 2016; Limberger et al., 2018). To better define the volume of the reservoir in this deterministic approach many authors improve the workflow using 3D geological models to better determined the volume of the aquifers for then globally applying the deterministic HIP approach (Bär, K., Sass, I., 2014; Yang et al., 2015). More recent and rigorous approaches have been implemented in the framework of nationwide projects in Netherlands (ThermoGIS project) and in specific parts of Italy (VIGORThermoGIS) which used 3D subsurface models and mapping techniques by means of Geographic Information Systems (GIS) to spatially and stochastically assess deep geothermal potential (Van Wees, et al., 2010, Kramers, et al., 2012; Trumpy et al., 2016). The codes behind these two tools are a reference for the geoscientific community and shape the way forward to assess resources on a regional scale. These tools make it possible to develop maps to show the HIP spatially, an essential aspect so that later, users, using GIS tools, can analyse the correspondence between the availability of resources and the location of demand. However, these tools are not designed to be used outside of the areas for which they were developed. Therefore, with the aim of having a standard and free access tool for the entire geothermal community that allows the calculation of HIP and heat recovery based on 3D data through Monte Carlo simulations, in February 2020 the Institut Cartogràfic i Geològic de Catalunya (ICGC) released a new free software called 3DHIP-Calculator (Piris et al., 2020). The new tool allows to assess the regional deep geothermal potential from the three-dimensional point of view using stochastically the volumetric USGS method. Using it, the user imports their own 3D geological and thermal models prepared before to evaluate their own case studies and derive maps. This new tool presented in the framework of the 8th EGW (European Geothermal Workshop) that took place from 7-8 October 2020 (online) will also be used within of the GeoERA H2020 Era-Net (Establishing the European Geological Surveys Research Area to deliver a Geological Service for Europe) HotLime project (Mapping and Assessment of Geothermal Plays in Deep Carbonate Rocks - Cross-domain Implications and Impacts).

The HotLime project, which will run from July 2018 to June 2021, is one of 15 projects approved under the GeoERA umbrella that has received funding from the European Union's Horizon 2020 research and innovation programme. The project focused on mapping, characterization and comparison of geological situations, in 11 deep carbonate reservoirs across Europe. The project is participated by 15 European geological survey organizations. The aims are to identify and apply uniform workflows for estimation deep hydrothermal resources in carbonate reservoirs. The principal outcomes will be spatial representations of the areas under investigation (3D models, 2D maps). Among the different case studies, one of them is situated precisely in the NE part of Catalonia (Spain) within the before mentioned named Empordà Basin. This case study assesses the low enthalpy geothermal resource in the lower Tertiary fractured limestone aquifer.

With the aim to perform a new an accurate resource assessment for the whole aquifer within the Empordà basin, new exploration campaigns, laboratory petrophysical analysis, and finally a new 3D geological, geophysical and thermal models have been coordinated and realized by ICGC within the period 2018 - 2020 with some specific support of the Autonomous University of Barcelona (UAB) and University of Barcelona (UB).

2. THE EMPORDÀ CASE STUDY (NE CATALONIA) - GEOERA HOTLIME PROJECT

2.1. The geological, hydrogeological and geothermal setting

Catalunya (Spain) is located in NE of Iberian Peninsula (SW of EU). The main structural areas within its territory are related to the Pyrenees ranges, the Southern Pyrenean foreland Basin (Ebre basin, the Catalan Coastal Ranges, and the Neogene basins such as the Empordà basin (EB) (Figure 1). The EB is a Neogene basin located in the NE of Catalonia, close to the Pyrenees ranges. It was generated during the opening of the 'Valencia Trough' (Late Oligocene – Middle Miocene) as the prolongation of the European Cenozoic Rift System. Due to extensional tectonics, EB was formed as a tectonic graben by a NW-SE-trending fault system, which overlaps the contractional structures of Alpine period (Saula et al., 1996). EB is internally cut by normal faults with listric geometry and measured dip slips of about 1000 m in the main ones. This faulting caused a blocky structure in the pre-Neogene bedrock, which presents a general deepening towards the north (Figure 3).

Within the lithostratigraphic succession from the Paleozoic to the Paleozene, a potential hot limestone aquifer was detected. It corresponds to the well-known Girona Limestone Formation (GLF), located in the Lower Eocene part of the sequence. Its thickness values range between 22m to 200m with a median of 75m. It shows an increase from E to the W (Pallí, 1972). Towards the N and in depth, the thickness increases to 270 m, according to interpreted cross-sections. The maximum depth reaches the 2650 m in the study area. The aquifer covers an area of more than 400 km².

Two deep wells exist in the area of study (Figure 1).

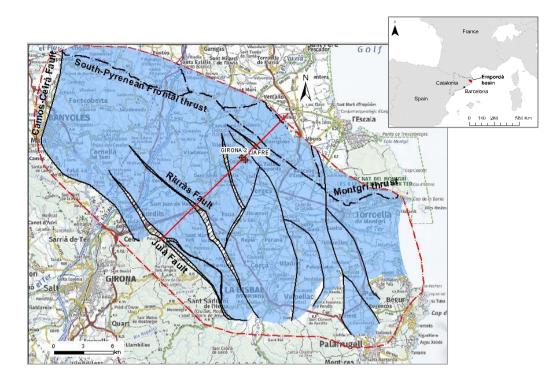


Figure 1: A) (top right) Location of the area of study within Europe. B). Area of the Empordà basin with the location of the main regional faults, according to ICGC (2017).

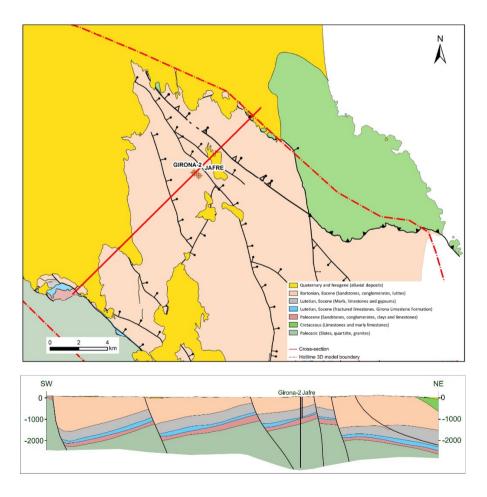


Figure 2: A) (top) Synthetic structural and lithological map of the study basin (modified from ICGC, 2014). The map shows the cross-section and the location of the borehole data used to build the 3D geological model; B) (below) Synthetical cross-section showing the location of the Girona Limestone Formation (GLF).

The first well called 'Girona-2'was drilled in the 1962 with a depth of 3319 m in the framework of the oil and gas exploration campaign within the Empordà basin. During the drilling campaign, it was observed that the fractured limestone aquifer located at a depth of 964m could have geothermal interest. The well showed artesian behaviour, with almost constant flowrate of 3-4 L/s, WHT (well-heat temperature) @ 48°C and with a fluid supersaturated in CO₂. Today, this well is clogged and unusable.

The second one it corresponds the geothermal "Jafre well" drilled in 1988 with a depth of 970 m near the town of Jafre. This new well drilled the same fractured limestone aquifer attributed to the base of the Tertiary (Girona Limestone Formation, GLF). It confirmed the geothermal potential observed with the old Girona-2 well from 915m to 968 m deep. It also showed the same artesian behaviour and a geothermal fluid at WHT@51°C with a constant artesian regime, and BHT@53,5°C. Interest in the 'Jafre' well was launched again in the 2000s, thanks to a private investment with the aim of promoting a new hotel-spa (PH, S.A. 2003). The well was reopened, and new hydraulic tests were carried out. However, this project was also abandoned for economic reasons a few years later.

The hydraulic parameters of the reservoir were interpreted in the 'Jafre well' by means of a well pumping test done over 14 days in March 2003 for the reopening project Two flow rate steps were used: 25 L/s (8.04 days) @ 51.6° C and 50 L/s (1.5 days) @ 51.7° C with the corresponding recovery periods. The aquifer behaved as a confined aquifer with an estimated BHP of 90 bar at steady state. Considering a thickness of 25 m in Jafre well, and an isotropic and homogeneous aquifer, the short-term analysis of the pumping test suggested the transmissivity, hydraulic conductivity and Storativity reservoir values of 100 m²/d (1.7e-3 m²/s), 4m/d (4.6e-5 m/s) and 3e-04, respectively which would correspond to a medium to low permeability fractured rock reservoir. More recently, laboratory results obtained by ICGC-UB (2019) from rock samples suggest that matrix is very low in between 0.2 to 0.01 mD. However, the analysis of the outcrops shows that the rock has a relatively high fracture density, likely allowing the GLF behaving as a fractured reservoir.

Despite the hopeful permeability values obtained in the short-term analysis (PH, S.A. 2003), the interpretation of the s/t curves at long-term also showed that, at least in this part of the basin (as can be observed in Figures 2 and 3), the aquifer is compartmentalized due to the presence of faults that can act as very low permeable geological boundaries. In this context, the aquifer capacity in the Jafre well study area should be considered moderate to low. Contrary, it is estimated that towards the west of the basin, the compartmentalization in the deeper parts of the aquifer could be less according to the current geological knowledge and the transmissivity higher due to a higher aquifer thickness. Regarding the reservoir porosity, the new data obtained by ICGC-UB (2019) indicates the rock matrix values are between 1 to 15%. In the other hand (PH, S.A. 2003) reported a value of 7.6% estimated from density-neutron logs. In this context, the fractures must play and important role increasing the secondary porosity. Regarding hydrogeochemistry, the fluid in the reservoir presented slightly acidic average pH values around 6.4, EC of 4575 μ S/cm.

Considering the BHT corrected values, for the Girona-2 well it was estimated the temperature gradient of the aquifer is 47°C/km. According to the BHT Jafre values, a geothermal gradient of 42°C/km measured from the top of the aquifer could also be considered, considering a mean annual surface temperature of 16°C. Until now, no geothermal resource assessment of the aquifer has been carried out at regional scale. Within the framework of the HotLime project, a new map of deep geothermal potential at regional scale using the classical Heat-in-Place method has been prepared using a probabilistic approach. The geometry of the aquifer obtained from the 3D geological model elaborated within the GeoERA HotLime project, will also allow a better re-interpretation of the tests in the future to provide a new more accurate evaluation of the resource at the Jafre location.

The main aim of the work is to generate the most probable 3D geological model of the aquifer which should honour all the available data. The resulted 3D probabilistic geological model is then used to construct a 3D thermal model. The workflow used must deal with the uncertainty of the aquifer geometry, so a stochastic approach was applied. The approach considers the construction of a first geological model that is then validated from geophysical methods that use potential fields such as gravimetry through geophysical inversion and following a full gravity litho-constrained stochastic approach. As the amount of gravity data was not enough, a new geophysical campaign was planned to complement them.

2.2. Geophysical exploration

The new campaign performed by the Geophysical Techniques Unit Team of ICGC consisted in the realization of measurements of the relative gravity along with the detailed location with a differential GPS (Trimble R8s) that measured the Real-time kinematic (RTK) positioning using the GNSS (Global System of Satellite navigation) system. The field campaign was carried out in the months between December 2018 and April 2019 with a total of 453 gravimetry measurements which include the measurements in the gravimetric bases, the repetitions of quality control of the campaign (6% of the total data) and the measurements themselves (365 observable) of the study area.

2.3. Petrophysical characterization

A new field campaign was also done by the University of Barcelona, to collect rock samples and characterize the outcrops analogues. The sampling campaign was oriented to characterize the carbonate facies of the reservoir. Afterwards the rocks samples properties were determined by laboratory test which includes, a: 1) petrological analysis of rock samples, using a Zeiss Axiophotop optical microscope with EC Plan-NEOFLUAR lenses and Euromex sCMEX-20 image sensor associated with the Dept.'s Euromex ImageFocusAlpha image capture and processing software; 2) determination of petrophysical parameters such specific heat capacity, thermal diffusivity, thermal, conductivity (in wet and dry conditions), density, porosity and hydraulic conductivity. For the thermal properties, a QuicklineTM-30 analyser Anter Corporation equipped with a probe of Applied Precision covering the range of 0,3 - 6 W/mK. The density was determined using a Cobos D-600 precision balance. The matrix porosity was determined by means of a helium porosimeter Jones S/N 9501. The permeability was determined under atmospheric conditions (nitrogen permeameter Jones S/N 9501) and confined conditions in eight samples (triaxial press TRI-X 250/200 Sanchez Technologies)

2.4. The 3D geological and geophysical model of the Empordà basin (NE, Catalonia, Spain)

The construction of the new 3D voxel based geological-geophysical and thermal model (sub-chapter 2.5) were built by the Hydrogeology and Geothermal Unit of the ICGC. The general workflow used for preparing them, which is presented more extensively by Herms et al (2020), was previously implemented as a test case in the Neogene basin of Reus-Valls (South, Catalonia).

To prepare the 3D geological model it was used a combination of three software: the 3D Kinematic MOVE Software (version 2019.1.2 Midland Valley) to construct some geological surfaces and new cross-sections; the SKUA-GOCAD software (version 15.5. Paradigm) to build the 3D surface-based model for then build the 3D voxel model; and the 3DGeoModeller software (version 4.0.5., Intrepid Geophysics) to apply stochastic techniques during the 3D geological model construction to compute the probability for each grid cell to belong to a specific lithostratigraphic unit and to better deduce the rock properties distributions needed to explain the geophysical observations (Husson, et al., 2018). This stochastic procedure allows the validation of the model. To address it, the preliminary geological 3D voxel model was exported to the 3DGeoModeller software. The validation was performed back and forth according to available geophysical potential-field data (gravity) by means of forward modelling and 3D geophysical inversion following a lithological-constrained stochastic gravity inversion. Therefore, in this stage, the rock densities values following a probability density function must be considered (Table 1, source: ICGC-UB, 2019, Cermak V. et al., 1982; Schön, J.H., 2011; Eppelbaum, L. et al., 2014; Bär, et al. 2019) for each geological model unit (i.e. a Gaussian distribution specifying the mean and the standard deviation). The steps are repeated until a good fit is achieved between the observed gravity data and the gravity modelled response. Previous studies about interpreting the 2D gravity response of the Empordà basin were also consulted (Rivero, et al. 2001).

The final model covers the area of the Girona Limestone Formation aquifer (400 km^2) at the south part of the Empordà Basin at the south of the south-Pyrenees frontal trust (the northern limit of the study area) and has a depth of 7km. This depth was established as the bottom boundary condition for the thermal model. At this depth, a temperature previously calculated from a lithospheric-scale purely conductive heat transport model implemented in the LitMod3D software will be applied (Fullea, et al. 2009).

The model of the Empordà basin consists of the following units of the stratigraphic model: Quaternary and Neogene (alluvial deposits); Bartonian, Eocene (Sandstones, conglomerates, lutites); Lutetian, Eocene (Marls, limestones and gypsums); Lutetian, Eocene (fractured limestones. Girona Limestone Formation), Paleocene (Sandstones, conglomerates, clays and limestones); Cretaceous (Limestones and marly limestones) and Paleozoic (Slates, quartzite, granites). The geological model is based on different data (Figure 3A): lineations and contacts from geological maps at scale 1:25.000 (ICGC, 1995, 1005, 1995b, 1997, 2001 and 2003); dip/azimuth measurements; the Girona-2 and Jafre well data; geological cross-sections, some geological surfaces from the 3D surface-based geological model of Catalonia (ICGC, 2013), and the major faults of the Main Structural Units of Catalonia (ICGC, 2017).

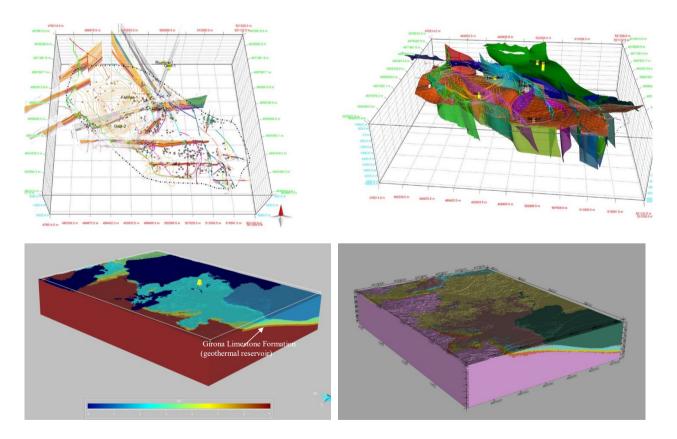


Figure 1: A) (top-left). Integration of available geological information at the first stage. B) (top-right). Preliminary 3D surface-base geological model. C) the preliminary 3D Voxel geological model and D) the 3D model used for the lithoconstrained geophysical inversion.

The final 3D model allows to obtain the aquifer thickness map and the map of the depth to aquifer top (Figure 4). As can be seen in these maps, the aquifer is highly compartmentalized due to regional faults. In this sense the old Jafre and Girona-2 wells were situated in a very unfavourable position in terms of geothermal exploitation. The geothermal conditions of the aquifer towards the west and in the deeper parts of the basin could be better as the aquifer thickness could reach higher values increasing therefore its hydraulic transmissivity. The aquifer deepens to the west and north, lying below the south-Pyrenees frontal trust.

Table 1: Loaded rock densities probability density functions in the 3DGeomodeller during the geophysical inversion step. (Mean value / Std. Standard deviation value).

Lithostratigraphic modelled	Geophysical inversion Density (g/cm ³)			
Geological age	Lithologies	Geothermal targets	Mean	Std
Quaternary and Neogene	Alluvial deposits	-	2.450	0.050
Bartonian, Eocene	Sandstones, conglomerates, lutites	-	2.630	0.050
Lutetian, Eocene	Marls, limestones and gypsums	-	2.615	0.050
Lutetian, Eocene	Fractured limestones (GLF)	The target reservoir	2.650	0.050
Paleocene	Sandstones, conglomerates, clays and limestones	-	2.575	0.050
Cretaceous	Limestones and marly limestones	-	2.710	0.050
Paleozoic	Slates, quarzites and granitoids	-	2.720	0.050

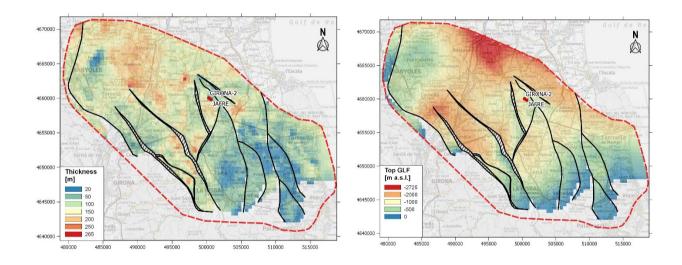


Figure 4: Outputs maps derived from the geological model: A) (left). Thickness of the fractured limestone Tertiary aquifer – Girona Limestone Formation. B) (right). Depth of the top of the fractured limestone Tertiary aquifer.

2.5. The 3D thermal model of the Empordà basin (NE, Catalonia, Spain)

Once the 3D geological model was finished, the next step was to build the 3D thermal model. In this case, a conduction dominated assumption was considered for the heat regional heat transport and steady state. To model the isotherm distribution, it was used the 3DGeoModeller software using the "*Forward Model Temperature*" module. The bottom and top boundary conditions used was the Dirichlet type (fixed temperature) with 151°C and 16°C (average surface temperature) respectively. No heat flux was considered by the lateral boundaries of the model. To consider the uncertainty of the thermal parameters (i.e. thermal conductivity (W/m·K) and heat production rate (W/m³), it was used, in batch, the called *Parameter Sweep - Heat resource uncertainty* algorithm. This algorithm solves the heat transport equations in steady state considering conduction and it calculates the isotherms for the entire domain following a quasi-stochastic approach (Intrepid-Geophysics, 2020). Therefore the algorithm considers for each geological model unit a probability density function (in this case a Gaussian distribution) defining the mean and the standard deviation (Table 2, source: ICGC-UB, 2019, Cermak V. et al., 1982; Vila, et al., 2010; Schön, J.H., 2011; Eppelbaum, L. et al., 2014; Bär, et al. 2019). Thus, all the elements of the simulation with no zero standard deviation can be perturbed along the simulation generating different 3D thermal models. Unlike a conventional full stochastic approach where n random values are taken from a distribution, the Parameter Sweep algorithm consider each variable as the mean, and standard deviation for each lithology independently.

A parameter sweep automatically creates many scenarios, running different simulations. All elements (physical properties defined by the user for each geological unit) of the simulation can be perturbed, so they are cycled through 2 or 3 states, making a combination of simulations that constitutes a stochastic study of the uncertainties. For instance, with 12 variables such as a unit's Heat Production Rate, and thermal conductivity for each geological model unit except the Girona Limestone Formation, each with 2 states gives 4096 cases. In this case 3 states would mean to much computing effort. Finally, 3DGeoModeller compile in a unique model all these 3D thermal models' solutions. The way to compile the different results is calculating the mean and Sd for the solutions distribution, i.e.,

for the 3^n models. The final 3D thermal model is shown in the Figure 5. The results fit well with the temperature values of the Girona-2 and Jafre well with errors below 0.2°C. The final 3D geological model and thermal models were exported as 3D voxel-based models in ASCII format which will contain the following data: the reservoir inferred temperature, the lithology, the voxel position (X,Y,Z coordinates) and the rock densities (derived from the geophysical inversion process).

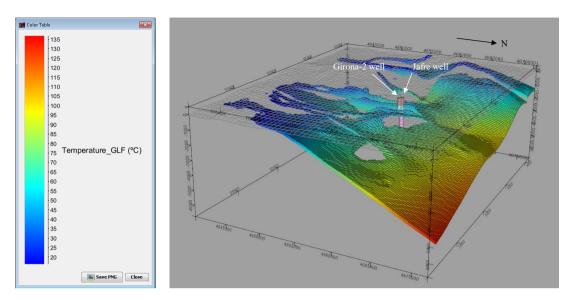


Figure 5: 3D Thermal model built upon 3DGeomodeller (screenshot)

Table 2: Loaded rock thermal properties probability density functions in the Parameter Sweep algorithm - Heat resource uncertainty algorithm of 3DGeomodeller. (Mean value / Std. Standard deviation value)

			Thermal model				
			Thermal conductivity Heat Product		uction Rate		
Lithostratigraphic modelled units			λ (W/mK)		HPR (HPR (W/m ³)	
Geological age	Lithologies	Geothermal targets	Mean	Std	Mean	Std	
Quaternary and Neogene	Alluvial deposits	-	1.60	0.50	1.10E-06	9.19E-08	
Bartonian, Eocene	Sandstones, conglomerates, lutites	-	1.85	0.20	1.20E-06	6.60E-07	
Lutetian, Eocene	Marls, limestones and gypsums	-	2.10	0.50	8.00E-07	5.00E-07	
Lutetian, Eocene	Fractured limestones (GLF)	The target reservoir	2.80	0.30	4.77E-07	3.56E-07	
Paleocene	Sandstones, conglomerates, clays and limestones	-	2.91	0.55	1.19E-06	6.60E-07	
Cretaceous	Limestones and marly limestones	-	2.37	0.52	4.77E-07	3.56E-07	
Paleozoic	Slates, quarzites and granitoids	-	3.50	0.50	2.20E-06	2.53E-07	

2.7 The geothermal resource assessment using 3DHIP-Calculator software

To assess the deep geothermal potential for the geothermal target (i.e. the Girona Limestone Formation aquifer), the volumetric Heat in Place (HIP) method (Muffler and Cataldi, 1979) was applied at each voxel from the resulted 3D voxel-based model using the 3DHIP-Calculator software (V 1.0. February 2020) which apply the Eq (1):

accessible resource base = HIP = V *
$$C_{\nu}$$
 * $(T_R - T_r)$ = V · $[\phi \rho_W C_W + (1 - \phi)\rho_R C_R] \cdot (T_R - T_r)$ Eq (1)

Where:

- HIP is the "heat in place", stored heat or accessible resource base (kJ)
- *V* is the volume of the aquifer (aquifer * thickness). For the 3DHIP-Calculator it represents the volume of the cells or voxels [m³] in the 3D voxel model that has been defined to discretise the reservoir.
- ϕ is the effective porosity [-]
- ρ_{w} , ρ_{R} is the density of the fluid and the rock [kg/m³]
- C_v is the volumetric heat capacity in the reservoir [kJ/m³ °C], where C_v [kJ/m³ °C], = c (kJ/kg°C) * ρ (kg/m³)
- C_w, C_R is the specific heat capacity of the fluid and the rock [kJ/kg·°C]
- *Tr* is the cell or voxel temperature [°C]
- Ti is the reinjection, abandonment temperature [°C] (as the threshold of economic or technological viability), the ambient temperature, (i.e. the annual mean surface temperature value) or other criteria such as the e.g. Limberger, et al. (2018); $Ti = Ti + 15^{\circ}$ C. where Ti is the annual mean surface temperature value.

The HIP method combined with probabilistic Monte Carlo simulations allows considering the reservoir uncertainties or heterogeneities as for example the porosity, rock density or the specific heat. In order to considerate it, for each parameter it can be

defined by a probability distribution functions (PDF) (e.g. the options of normal, or triangular in the 3DHIP) and the HIP result can be evaluated by a probabilistic way obtaining a new PDF from which the P10 (very low confidence of the estimation and high values), P50 and P90 (high confidence of the estimation and low values) can be extracted.

The resource assessment was done with the new 3DHIP-Calculator tool, by the Hydrogeology and Geothermal Unit of ICGC in collaboration with the Unit of Geotectonics of the Department of Geology, Faculty of Science of UAB. The new 3DHIP-Calculator software (v1.0 February 2020) written in MATLAB (version 2019) and delivered and distributed in a compiled executable program for Microsoft Windows[™] (3DHIP-Calculator.exe). The 3DHIP-Calculator software is free downable from the ICGC website. It has an intuitive graphical user interface (GUI) that help their utilization. The results are presented in different graphs (histograms and cumulative probability functions) and 2D maps. The output data can then be exported to Geographic Information Systems (GIS) for more detailed 2D mapping to show probabilities of the available resource (for example, 10% HIP (P10)), HIP (P50) or HIP (P90).

Table 3: Parameters introduced at the 3DHIP-Calculator.

Heat in Place	Units	mean	std.	probability distribution	
Thickness of the reservoir (calculated for each voxel *)	m	-	-	-	
Area of the reservoir (calculated for each voxel *)	m²	-	-	-	
ρ_r = rock density (calculated for each voxel *)	kg/m ³	-	-	-	
Ø = Porosity	-	0,055	0,031	normal	
Cr = Specific heat capcity (rock) at reservoir condition	kJ/kg°C	0,86	0,10	normal	
Ti = Temperature of the reservoir (°C) (calculated for each voxel **)	°C	-	-	-	
$\rho_{\rm w}$ = fluid density (kg/m ³);	kg/m ³	962,18	0,18	normal	
Cw = specific heat capacity (fluid) at reservoir condition	kJ/kg°C	4,17	4,22	normal	
Tf = Reference temperature (°C)	°C	26,00	-	fixed value	

(*) values estimated during the geological 3D model validation by the geophysical stochastic inversion

(**) values estimated for the 3D thermal model. Parameter sweep analysis.

The results from a Monte Carlo Simulation is presented as a histogram of number of occurrences of a particular value (Probability Density Function - PDF) and as a plot of the Cumulative Distribution Function (CDF).

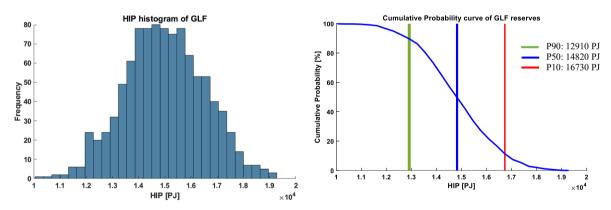


Figure 6: A) (left) Probability curve of HIP in the Empordà Basin for the Girona Limestone Formation. B) (right). Cumulative probability curve with the indication of the P10, P50 and P90.

The values of the total estimated stored heat (HIP) in the aquifer reported by the 3DHIP-Calculator are: 12910 PJ (P90, high confidence); 14820 PJ (P50, medium confidence) or 16730 PJ (low confidence).

The results obtained with 3DHIP-Calculator allowed to derive the HIP maps at the aquifer local scale. This document presents the preliminary results achieved and discusses the lessons learned within the framework of the project. The final maps presented in this work have been prepared using the free and open-source cross-platform desktop GIS application QGIS (version 3.12.2 'București'. To obtain the raster maps, the HIP values in the 3D-grid are vertically summed.

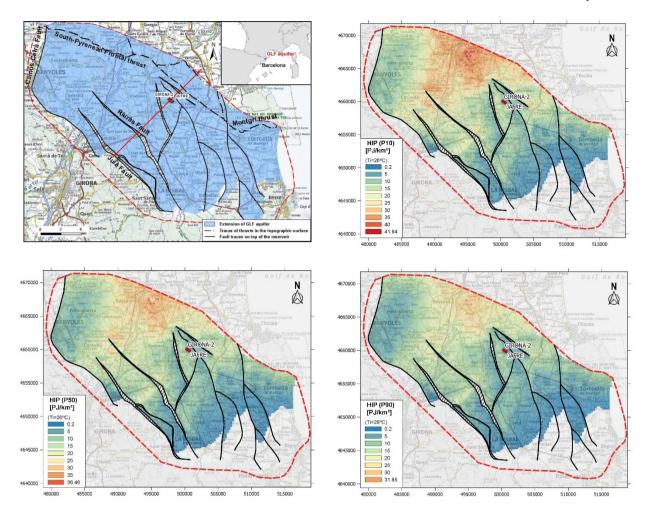


Figure 7: A) (top left) Extension of the GLF aquifer with the main faults. B) (top-right) HIP map P10. C) (bottom-left) HIP map P50 and D) (bottom-right) HIP map P90.

The wellhead thermal energy or theorical recoverable energy (H_{rec}) in terms of energy (Joules) can be simply related to the HIP in the reservoir by the recovery factor, R_g , (Eq 2 and 3) (Williams, 2004). H_{rec} can be also estimated with the Eq (4). Assuming a volume drained by a theorical well pumping the aquifer, we can infer the Rg by substituting Eq (4) and Eq (1) in the Eq (2), getting Eq (5).

$$R_{g} = H_{rec} / HIP \qquad Eq (2)$$

$$H_{rec} = HIP \cdot R_g$$
 Eq (3)

 $H_{rec} = m_w * (h_w - h_{ref}); \text{ where for simplicity; } m_w = V * \emptyset * \rho_W$ Eqs (4)

$$R_g = \frac{\mathbf{V} * \mathbf{\emptyset} * \mathbf{\rho}_{\mathbf{W}} \left(h_w - h_{ref} \right)}{\mathbf{V} * C_v * (\mathbf{T}_{\mathbf{R}} - \mathbf{T}_{\mathbf{r}})}$$
Eq (5)

Where:

- Hrec is the expected recoverable heat energy (kJ) at the well head considering a Rg
- R_g recovery factor at the well head [-]
- m_w is the extractable mass in the well [kg]
- h_w enthalpy of the produced fluid at T_R and $P_R = 224$ [kJ/kg]
- h_{ref} enthalpy of reference temperature at T_R and $P_R = 109,11$ [kJ/kg]
- P_R pressure at the reservoir @ 910 m = 91,6 [bar]
- P_R pressure at ambient conditions @ 0 m = 1,03 [bar]

The Eq (5) is applied for the conditions of the in the Jafre well (PH, S.A. 2003), considering a sustainable water flow rate of 17 L/s for 1 year. The radius of influence of the pumping (without considering recharge) is estimated by the Eq (6)

$$R = \sqrt{\frac{Q * t}{\phi * b * pi}}$$

Where:

- R radius of influence of the pumping = 352,3 m
- Q water flow rate = $17 \text{ L/s} = 1468.8 \text{ m}^3/\text{s}$
- t time = 1 year
- ϕ is the effective porosity [-] = 0,05
- b net thickness = 25 m (in Jafre well)

The HIP (Eq 1) contained in the affected volume due to the pumping, considering R area and b; is 0,5905 PJ. The H_{rec} (Eq 4) extracted by the well at Q and pumping t time is 0,0610 PJ. Therefore, the R_g estimated by the Jafre well is:

$$R_g = 0,0610 / 0,5905 = 0,103$$
 Eq (2)

According to Williams, et al. (2008), USGS resource assessment R_g for fracture-dominated reservoirs was estimated to range from 0.08 to 0.2, with a uniform probability over the entire range. For sediment-hosted reservoirs this range was increased from 0.1 to 0.25. The values obtained in this case considering the data coming from the Jafre well of 0.103, seems very consistent.

The obtained value of Rg = 0,103, is then applied for the whole aquifer, using the estimated HIP P10, P50 and P90 (Table 4).

Table 4: F	Estimated total	l Heat in Place ar	d Recoverable	Heat in the Girona	Limestone Formation aquifer
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		Heat in Place	Rg	Recoverable Heat	
		[PJ]		[PJ]	[GWh]
P90	high confidence	12910	0,103	1329,73	3,69E+11
P50	medium confidence	14820	0,103	1526,46	4,24E+11
P10	low confidence	16730	0,103	1723,19	4,79E+11

3. DISCUSSION AND CONCLUSIONS

The USGS Heat In place method together with Monte Carlo Simulation is the most widely used method in early exploration stages. The methodology consists of combining probability density functions for uncertain estimates of the variables of the reservoir. A case study in the lower Tertiary fractured limestone aquifer within the Empordà Basin, located in the north-eastern sector of the untrusted foreland basin of the Pyrenees in NE Catalonia has been presented. The study was performed in the framework of the GeoERA HotLime project (co-financing H2020). A new 3D geological and thermal model of the reservoir-bedrock system was developed combining different software and methods and considering the uncertainty in all steps. Afterwards a 3D thermal model was prepared. Both models were used to perform the geothermal assessment aquifer delivering HIP maps of the entire reservoir. The geothermal potential assessment has been addressed using the new 3DHIP-Calculator tool (Piris, et al. 2020), a Matlab-based software compiled for Windows which allows to stochastically apply the Heat-In-Place method (Muffler and Cataldi, 1978, Muffler, L.J.P., 1979) by using 3D voxel models. The analysis of the named Jafre well, an old well drilled in 1988, confirms that the Recovery factor R_g would be around 0,103 within the range for fracture-dominated reservoirs between 0.08 to 0.2 according to Williams, et al. (2008). The results reported by the 3DHIP-Calculator indicate that the total estimated stored heat (HIP) in the aquifer are: 12910 PJ (P90, high confidence); 14820 PJ (P50, medium confidence) or 16730 PJ (low confidence). The theoretical recoverable energy considering the R_g factor 0,103 would be 1329,7 PJ (P90, high confidence); 1526,46 PJ (P50, medium confidence) or 1723,19 PJ (low confidence).

These obtained thickness and HIP maps have allowed to identify the most favourable and promising areas to go forward for the planning and development of new prospections at local scale. According to the final 3D model, it seems that the geothermal conditions of the aquifer towards the west and in the deeper parts of the basin could be better than in the Jafre location, from the following interpretations: the degree of aquifer compartmentalization due to regional faults (according to the structural map of the Figure 1) could be less, and the reservoir temperature, at the same gradient, could be higher. Consequently, the Jafre location, at the moment, does not appear to be the most interesting and promising area of the aquifer for a possible geothermal exploitation project, even though it is the only location in the aquifer where, to date, a deep well has been drilled for exploration.

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Eq (6)

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