Innovative and Sustainable Groundwater Management in the Mediterranean

D3.1 Selection of the Smart Model Types Suitable for Application to Groundwater Systems

VERSION 2.0

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Glossary

ANN	Artificial Neural Network.
BU	Boğaziçi Üniversitesi.
CERTE	Centre de Recherches et des Technologies des Eaux.
GA	Grant Agreement.
IST-ID	Associação do Instituto Superior Técnico para a Investigação e Desenvolvimento.
MED	Mediterranean.
MW	Monitoring Well.
NGO	Non-governmental organizations.
PU	Public.
R	Document, report.
RF	Random Forest.
RCM	Regional Climate Model.
RCP	Regional Climate Projection.
SPEI	Standardized Precipitation Evapotranspiration Index.
SPI	Standardized Precipitation Index.
SGI	Standardized Groundwater Index.
TUC	Technical University of Crete.
UFZ	Helmholtz-Zentrum für Umweltforschung.
UNIPR	Università degli Studi di Parma.
UPV	Universitat Politècnica de València.
WP	Work Package.

Executive Summary

The overall objective of the InTheMED project is to implement innovative and sustainable management tools and remediation strategies for MED aquifers (inland and coastal) in order to mitigate anthropogenic and climate-change threats by creating new long-lasting spaces of social learning among different interdependent stakeholders, NGOs, and scientific researchers in five field case studies. These are located at the two shores of the MED basin, namely in Spain, Greece, Portugal, Tunisia, and Turkey.

InTheMED will develop an inclusive process that will establish an ensemble of innovative assessment and management tools and methodologies including a high-resolution monitoring approach, smart modelling, a socio-economic assessment, web-based decision support systems (DSS) and new configurations for governance to validate efficient and sustainable integrated groundwater management in the MED considering both the quantitative and qualitative aspects.

This Deliverable aims to illustrate surrogate models and their applications for groundwater purposes. An extended scientific literary review was carried out to evaluate the most promising surrogate models. Three examples are presented in order to illustrate pros and cons of the surrogate models.

1. Overview

Stakeholders need simplified models, yet accurate enough, to analyse alternative scenarios and make decisions under uncertain future conditions. Aquifer numerical modelling has reached high levels of completeness and reliability. However, models, made by specialized software packages are complex to set up, have extensive data requirements, take long time to run, and require specialized personnel to perform the simulations and analyse the results. For this reason, InTheMED focuses on the development of new simplified "smart" models. These new models will be built on the basis of long-time historical data and/or detailed numerical models with the aim to provide specific answers tailored to the stakeholder needs. The smart and calibrated models developed in this way can also be used to analyse the effects of climate change and hypothetical scenarios of socio-economic activities that may induce a change in groundwater exploitation.

The choice of the most suitable models is closely linked to the purpose of the investigation and to the problem at hand. Several activities in order to complete Task 3.1 were carried out:

- scientific literary review of recent documents related to surrogate modelling in groundwater (Attachment A);
- development and analysis of a survey regarding the study sites (results are reported in the Milestone M3.1, see Tanda et al., 2021);
- identification of the best surrogate models suitable for pilot sites: artificial neural network (ANN), random forest (RF) and linear regression;
- application of ANN, RF to synthetic cases and linear regression to field data;
- presentation of the results (see Section 2) to project partners during the meeting of May 7th;
- discussion with each project partner regarding the case studies (Section 3).

Following, the results of the synthetic cases and of the meeting with project partners are reported.

2. Test cases

The goal of surrogate models is to achieve a rapid response following a stress. For example, the knowledge of the nitrate concentrations at monitoring wells (MWs) due to the spread of a fertilizer in a specific area is of primary importance. The surrogate models, once calibrated, allow the evaluation of different scenarios that consider, for instance, different releases.

Both ANN and RF (Figure 1) are promising approaches for surrogate modelling. To evaluate the applicability of these methods, two literary test cases were considered: the first deals with groundwater flow (effect of recharge and pumping rate on hydraulic heads at monitoring points) and the second with groundwater transport (estimation of concentrations at monitoring wells starting from different releases). Before the realization of the surrogate model, in order to solve flow or transport problems, various procedures must be performed. Since it is a data-driven surrogate model, observed data generation is required. Therefore, groundwater flow and transport numerical models have been applied for dataset generation. Inputs necessary for the numerical model, in order to reduce the number of forward simulations, are usually obtained by means of the Latin Hypercube Sampling (LHS) which represents a statistical method to randomly generate variable from a multidimensional distribution. Then, the generated dataset is divided into three different subsamples: training, validation and test dataset. By means of a learning process, the training dataset will be used to calibrate the network so that it would be able to provide the desired output. The validation set is used to verify that the training process does not generate overfitting, while the test set verifies the generalization capacity of the network.

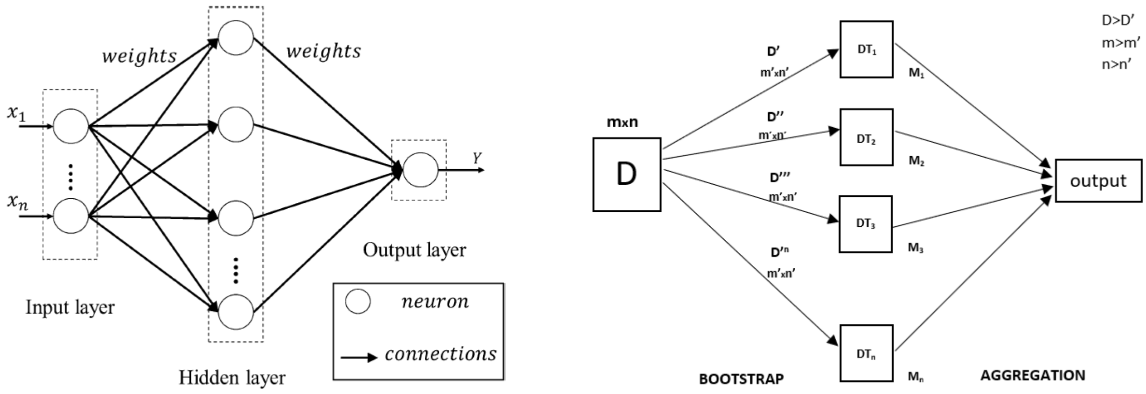

Figure 1 – (left) Scheme of Artificial Neural Network. (right) Scheme of random forest.

The last example deals with the effect of climate change on groundwater resource. A linear regression model is applied to project future groundwater levels using historical rainfall, temperature and groundwater level data and climate models outputs.

2.1. Case 1: Groundwater Flow

The study case proposed by Hendricks Franssen et al. (2009) was considered. The test case consists of a confined aquifer of 5000 m×5000 m with 50×50 cells (Figure 2). The West and East boundary conditions are assigned hydraulic heads respectively of 0 m and 5 m, while the North and South are no-flow boundaries. The aquifer presents a surface recharge and a pumping well (Figure 2). The transmissivity field is Gaussian and was generated with an exponential variogram with $\sigma^2_Y = 1$ (where Y = ln(T)) and correlation length of 500 m (Figure 2).

The objective of the test was to reproduce hydraulic heads (output of the surrogate model) at monitoring wells knowing only the recharge rate and pumping well rate (inputs of the surrogate model). Both ANN and RF (Figure 1) were trained using data collected through the numerical modelling. In particular, the effects of several pumping well flow rate (0.02-0.095 m^3/s) and recharge rate (100-600 mm/y) were simulated. For a total of 176 forward simulations, the hydraulic heads at 25 monitoring wells were collected. The dataset has been divided in training (70%), validation (15%), and test (15%).

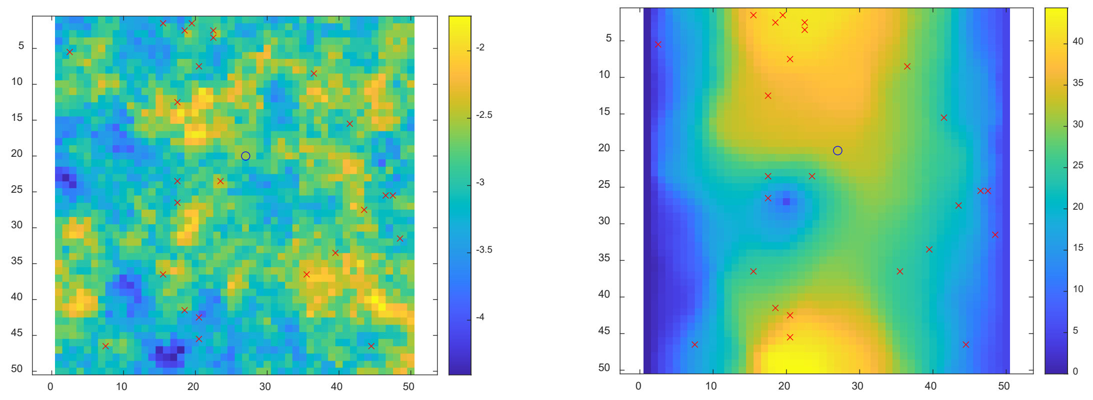

Figure 2 – (left) Synthetic example for groundwater flow. Each colour represents the natural logarithm of the transmissivity; (right) example of computed hydraulic heads in meters. The red crosses are monitoring wells and the blue circle denotes the pumping wells. Numbers on axis identify the cells.

Figure 3 reports the results obtained with the application of the two surrogate models. Both models can reproduce observed data with satisfactory accuracy.

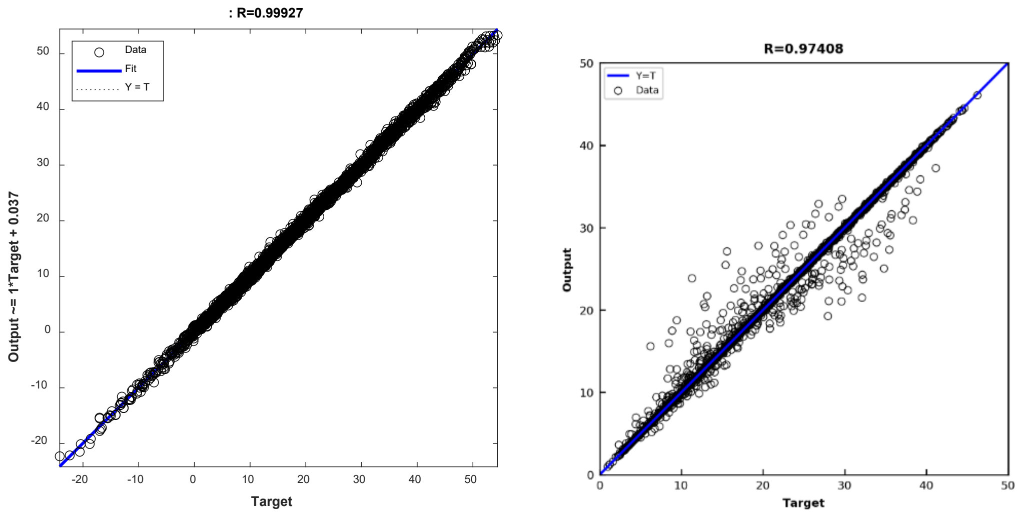

Figure 3 – (left) Observed-estimated hydraulic heads ANN approach. (right) Observed-estimated hydraulic heads RF approach.

2.2. Case 2: Groundwater Transport

To evaluate the performance of ANN and RF, a literature case introduced by Ayvaz (2018) and later adopted in Xing et al. (2019) and Jamshidi et al. (2020) has been considered. Figure 4 shows the discretization grid of the numerical model of the studied aquifer. See Ayvaz (2018) for hydraulic and geometry characteristics of the studied case.

The aquifer system consists of 5 different hydraulic conductivity zones whose isotropic conductivity values ranges from 0.0001 m/s to 0.0007 m/s. The conductivity values are taken as uniform inside each zone. The aquifer case dealt with a steady-state and non-uniform flow conditions; since the transport problem behaves ad an uncoupled problem, piezometric heads and velocity have been computed once. There is one active contaminant source and 7 monitoring locations in the aquifer domain (Figure 4). The total simulation time is 5 years divided into 10 stress periods of 6 months each. It is assumed that the source releases (input for the surrogate model) conservative compounds during the first 24 months (Figure 4). The concentrations at MWs (output of the surrogate model) were collected after 5 years of the starting of the release. Therefore, the contaminant transport process in the aquifer is transient. 256 samples of release mass rate located in the source and selected by means of LHS algorithm, run as forward simulations in order to compute contaminant concentration through the groundwater domain. Since the release mass rate and the concentration values are available by means of the numerical model, the surrogate model can be trained to estimate concentrations by knowing the release history. For the ANN computation, the dataset was divided in training (70%) and validation (30%). For the test phase a golden test has been used in order to compare the results obtained with the literature (Ayvaz, 2018).

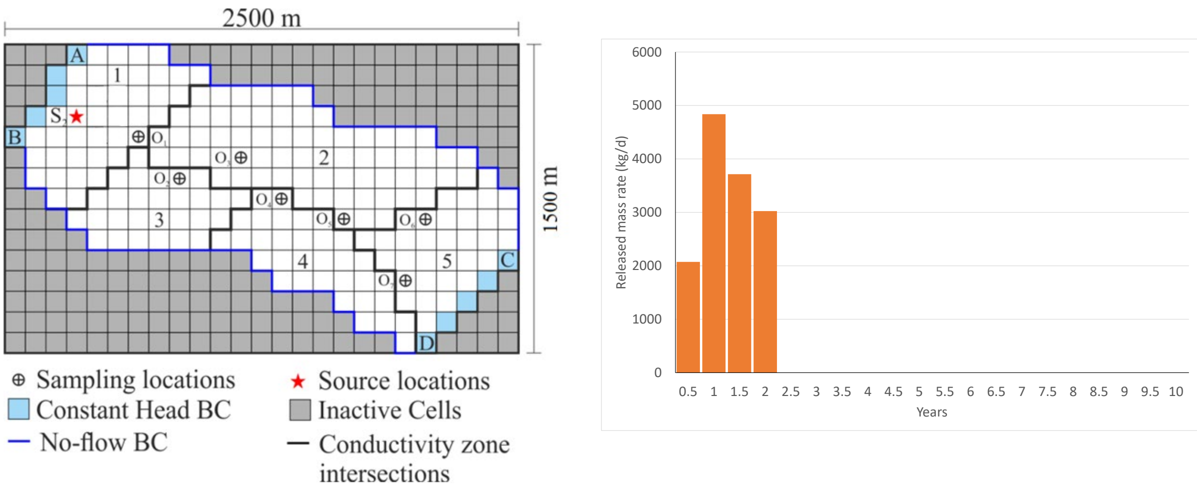

Figure 4 – (left) Numerical grid of the study case. (right) Released mass rate at source

A comparison of the results obtained through ANN and RF can be made analysing the Figure 5 and Figure 6 that show the observed and estimated concentration at MWs respectively. It is clear that both approaches well reproduce the true concentration values.

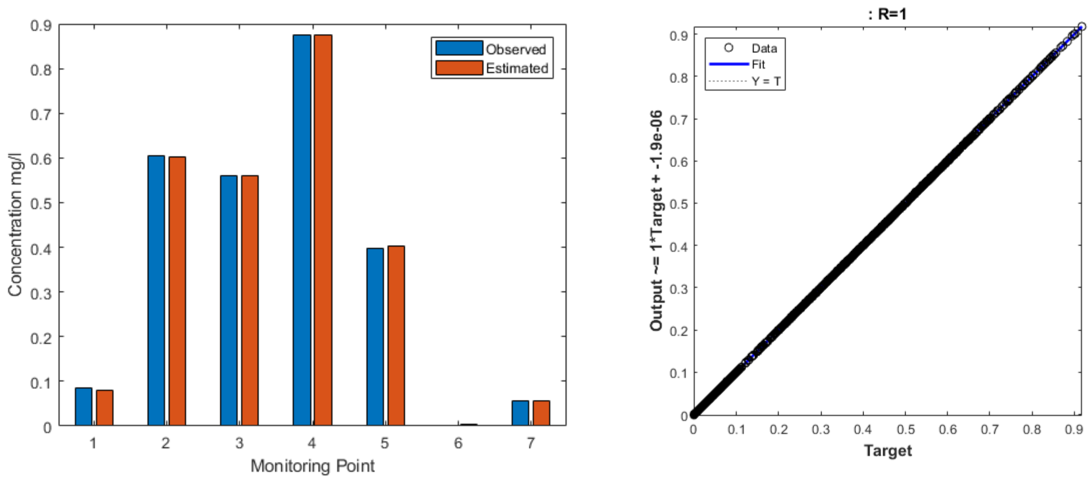

Figure 5 – ANN Observed and Estimated concentration at monitoring wells, forward simulation with one release source.

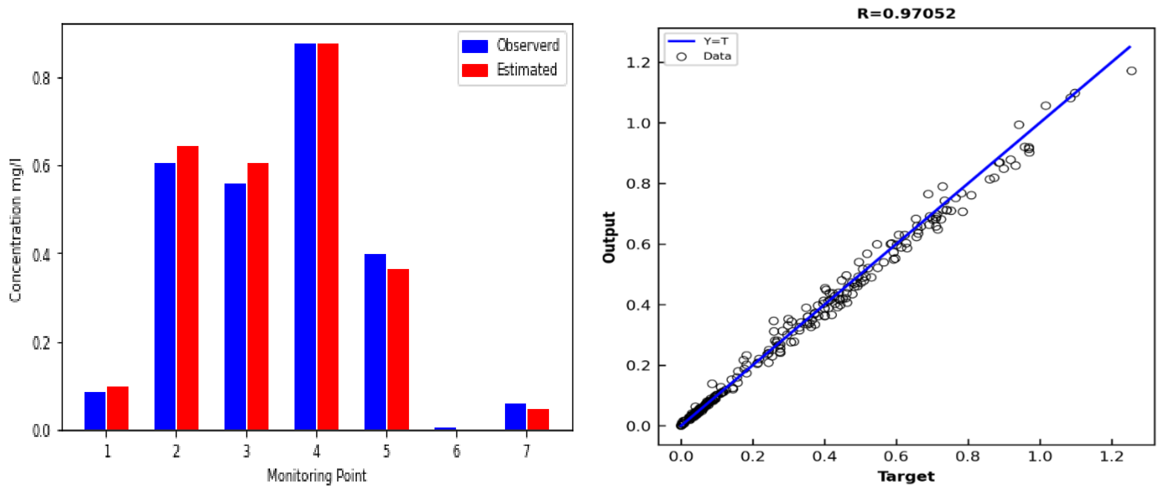

Figure 6 – RF (left) Observed and Estimated concentration at monitoring wells, forward simulation with one release source. (right) Observed estimated concentrations

2.3. Case 3: Linear Regression Approach

A linear regression approach has been applied to simple evaluate the impacts of climate change on groundwater levels (Secci et al., 2021). Possible correlations between the meteorological and groundwater indices have been examined making use of historical rainfall and temperature data and water levels collected in monitoring wells. The climate variables are investigated in terms of Standardized Precipitation Indices (SPIs) and Standardized Precipitation Evapotranspiration Indices (SPEIs); the groundwater levels are analysed with reference to the Standardized Groundwater Index (SGI). For those wells presenting satisfactory correlation, a linear regression relationship has been computed between SGIs and SPIs, and SGIs and SPEIs. The same relationships have been applied to future SPI and SPEI values, estimated by means of an ensemble of regional climate models (RCMs), to infer future SGI indices under different climate scenarios (RCP 4.5 and RCP 8.5). This methodology has been applied to data collected in Northern Italy (Secci et al., 2021), but the procedure can be easily applied to different areas of interest.

As an example, Figure 7 shows the couples SGI-SPI plotted together with the regression line and the identity line for a specific well (Paganico). The results for the Paganico monitoring well are presented in terms of box-plots of the SGIs obtained through the SGI-SPI (Figure 8a) and SGI-SPEI (Figure 8b) regression equations for the historical period and at short-, medium- and long-term under the two RCP scenarios.

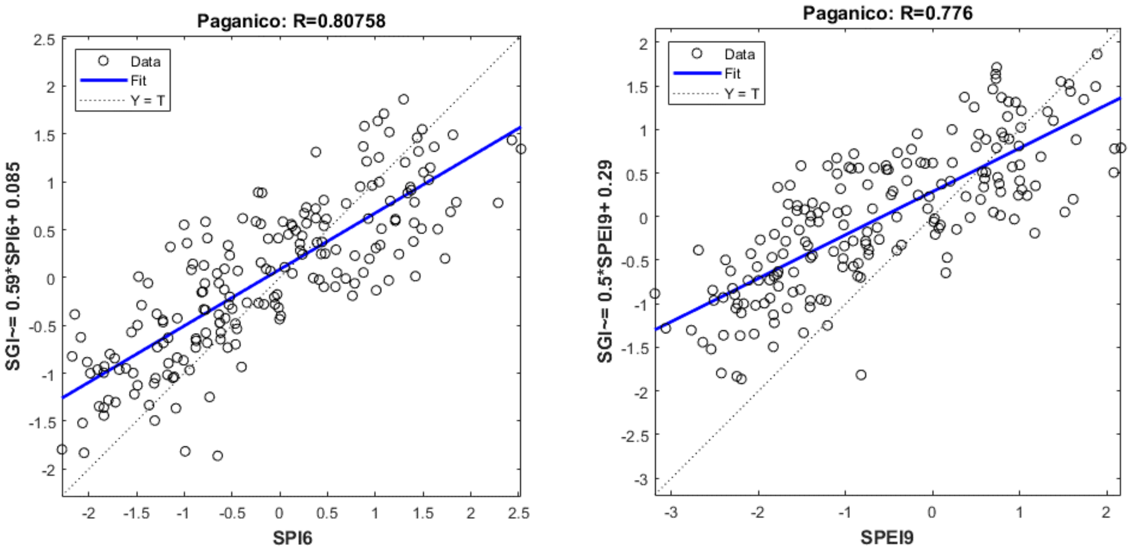

Figure 7 – SGIs versus SPIs (left) and SGIs versus SPEIs (right); the points represent the SGI data, the blue line indicates the regression line and the dashed line denotes the identity line. For each well, the correlation coefficient (R) and the regression equation is reported.

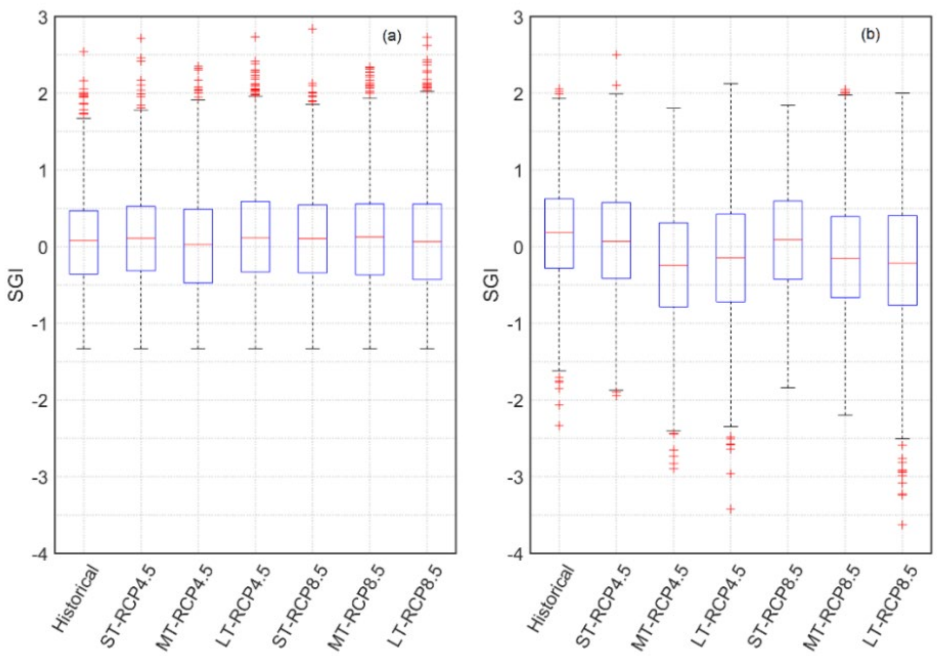

Figure 8 –Box-plots of the SGIs obtained for the Paganico monitoring well through the SGI-SPI (a) and SGI-SPEI (b) regression equations for the historical period and at short- (ST), medium- (MT) and long-term (LT) under the two RCP scenarios.

3. Virtual meetings with project partners

On May 7th, 2021 (14:30-16:30 CEST) all partners virtually met to discuss about surrogate models. UNIPR presented the results of the survey sent to partners in autumn 2020. The survey (results are reported in the Milestone M3.1, see Tanda et al., 2021) regarded the objectives of each site. Considering that all the study sites will investigate several scenarios of climate change; UNIPR presented a brief introduction on climate data and sea level rise. The survey allowed to distinct the sites into two groups: sites with numerical models (Requena - Utiel (Spain), Tympaki (Greece), Castro Verde (Portugal), Konya (Turkey)) and without (Grombalia (Tunisia) and Mediterranean Sea region).

In order to focus on each study case from July 7 to July 12, 2021 individual meetings with each project partners have been carried out. Following, the main outcomes are briefly reported.

Requena-Utiel (Spain)

The main objective of the surrogate modelling is to evaluate the groundwater drawdown taking into account different pumping, crop and climate scenarios. For this purpose, a surrogate model of the studied area based on Random Forest theory will be developed. UPV is improving a numerical groundwater flow model developed with MODFLOW in order to set up the surrogate model.

Tympaki (Greece)

The main goal of the surrogate modelling is to assess groundwater levels and nitrate concentrations in monitoring wells taking into account different pumping, crop and climate scenarios. TUC is developing a groundwater flow and transport model with FEFLOW to simulate the state of the art and provide data for the surrogate model. Artificial Neural Networks are suitable surrogate models for this problem.

Castro Verde (Portugal)

The objective of the pilot site is to forecast the depth of the water table under different climate scenarios. At this aim meteorological data, hydraulic heads at monitoring wells and pumping rate will be collected to set up a surrogate model.

Konya (Turkey)

The objective of the pilot site is to estimate the water budget for the entire basin and analyse the effects of different climate scenarios on water availability in the basin. At this aim a groundwater numerical model is under development and will be ready before the end of the year. The results of the numerical model and field data will be used to set up a surrogate model.

Grombalia (Tunisia)

The site is affected by groundwater contamination. The research group will focus on organic pollution and chemical oxygen demand (COD). CERTE will collect field data (such as rainfall, temperature, water depth, COD concentrations at MWs) and geological information in order to set up a surrogate model with a linear regression approach or with artificial neural network.

Mediterranean Sea Region

UFZ will perform trend analysis and clustering of groundwater quality and dynamic using the long-term time's series data collected from different Mediterranean countries. At this aim Random Forest and/or Artificial Neural Network will be developed.

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