Establishing the European Geological Surveys Research Area to deliver a Geological Service for Europe

Deliverable 4.2

PILOT DESCRIPTION AND ASSESSMENT

Permo-Triassic aquifer (United Kingdom)

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LIST OF ABBREVIATIONS & ACRONYMS

BGS	British Geological Survey
CC	Climate Change
EU	European Union
FAO	Food and Agriculture Organization
GCM	Global Circulation Models
GSO	Geological Survey Organization
ISIMIP	Inter Sectoral Impact Model Inter-comparison Project
NSE	Nash-Sutcliffe Efficiency
PET	Potential Evapo-Transpiration
R	Regression coefficient error
WP	Work Package

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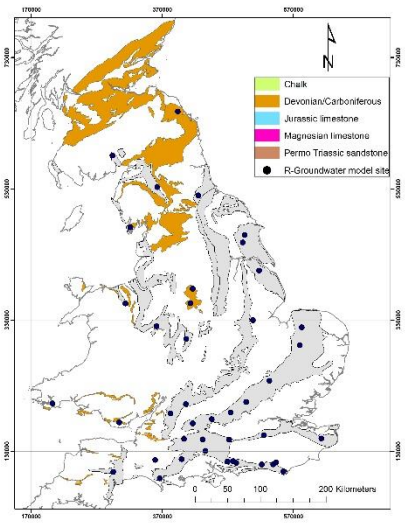
1 EXECUTIVE SUMMARY

Pilot name	Boreholes in the Devonian / Carboniferous Limestone aquifer	
Country	United Kingdom	
EU-region	North-western Europe	
Area (km^2)	NA	
Aquifer geology and type classification	Consists of Monitoring boreholes for water resources management up to 600 m thick. A possible yield up to 125 l/sec of good quality hard to moderately hard water from the upper parts of the aquifer.	
Primary water usage	Irrigation / Drinking water / Industry	
Main climate change issues	Risk of high precipitation causing increased river flows and flooding. Risk of drought.	
Models and methods used	Lumped groundwater modelling (AquiMOD). Transfer Function-Noise Model (Metran)	
Key stakeholders	Government. Research institutes. Water companies.	
Contact person	British Geological Survey. Andrew McKenzie	

This report describes the work undertaken by the British Geological Survey (BGS/UKRI) as a part of TACTIC WP4 to calculate historical and future groundwater recharge across the outcrop of Devonian / Carboniferous Limestone aquifer and at selected observation boreholes within these aquifers. Multiple tools, selected from the TACTIC toolbox that is developed undert WP2 of the TACTIC project, have been used for this purpose.

The Carboniferous Limestone aquifer in England and Wales include a wide variety of rock types that are fractured and well developed as aquifers in some areas. Where it is a major aquifer, the Carboniferous Limestone aquifer exhibit 'karstic' hydrogeological behaviour. The Devonian sediments of south Wales and the Welsh borderlands are continental deposits known as the Old Red Sandstone facies. In Scotland, the Devonian sandstones in Fife and eastern Scotland are one of the most productive bedrock aquifers in Scotland (Macdonald et al., 2005).

Three tools have been used to estimate the recharge values. These are the lumped parameter computer model AquiMod (Mackay et al., 2014a), the transfer function-noise model Metran (Zaadnoordijk et al., 2019), and the distributed recharge model is developed ZOODRM (Mansour and Hughes, 2004). Future climate scenarios are developed based on the ISIMIP (Inter Sectoral Impact Model Inter-comparison Project (www.isimip.org) datasets. The resolution of the data is 0.5°x0.5°C global grid and at daily time steps. As part of ISIMIP, much effort has been made to standardise the climate data (e.g. bias correction).

The estimation of the recharge model using the lumped model AquiMod is achieved by running the model in Monte Carlo mode. This produces many runs that are equally acceptable and consequently the uncertainty in the estimated recharge values can be assessed. The application of additional tools provides an additional mean to assess this uncertainty. Groundwater data at three boreholes are used in this model. The differences between the 75th and 25th percentile recharge values are found to be between 15% and 26%, which indicates a relatively high degree of uncertainty. In addition, the recharge values estimated using the distributed recharge model are found to be significantly higher than those estimated using the lumped model. It must be noted that the distributed recharge model calculates potential recharge while the lumped model calculates actual recharge. The absolute recharge values calculated by the transfer function-noise model Metran are also different from those calculated by the lumped model. The transfer function model estimates lower values at two boreholes and higher values at the third borehole.

Future recharge values calculated using the projected rainfall and potential evaporation values are -3.5 to 12.5% different from historical values on average. The 3o Max scenario, the wettest used in this work, produces values that are very different from the historical ones. This is observed in the output of both the lumped and the distributed models. Finally, future estimates are discussed in this report using long term average recharge values. It is recommended to carry out further analysis to these output in order to understand the temporal changes in recharge values in future, especially over the different seasons. In addition, it is recommended that the values and conclusion produced from this work should be compared to those obtained from different studies that applies future climate data obtained from different climate models.

2 INTRODUCTION

Climate change (CC) already has widespread and significant impacts on Europe's hydrological systems incuding groundwater bodies, which is expected to intensify in the future. Groundwater plays a vital role for the land phase of the freshwater cycle and has the capability of buffering or enhancing the impact from extreme climate events causing droughts or floods, depending on the subsurface properties and the status of the system (dry/wet) prior to the climate event. Understanding the hydrogeology is therefore essential in the assessment of climate change impacts. Providing harmonised results and products across Europe is further vital for supporting stakeholders, decision makers and EU policies makers.

The Geological Survey Organisations (GSOs) in Europe compile the necessary data and knowledge of the groundwater systems across Europe. To enhance the utilisation of these data and knowledge of the subsurface system in CC impact assessments, the GSOs, in the framework of GeoERA, has established the project "Tools for Assessment of ClimaTe change ImpacT on Groundwater and Adaptation Strategies – TACTIC". By collaboration among the involved partners, TACTIC aims to enhance and harmonise CC impact assessments and identification and analyses of potential adaptation strategies.

TACTIC is centred around 40 pilot studies covering a variety of CC challenges as well as different hydrogeological settings and different management systems found in Europe. Knowledge and experiences from the pilots will be synthesised and provide a basis for the development of an infrastructure on CC impact assessments and adaptation strategies. The final projects results will be made available through the common GeoERA Information Platform (http://www.europe-geology.eu).

The specific TACTIC activities focus on the following research questions:

- What are the challenges related to groundwater- surface water interaction under future climate projections (TACTIC WP3).
- Estimation of renewable resources (groundwater recharge) and the assessment of their vulnerability to future climate variations (TACTIC WP4).
- Study the impact of overexploitation of the groundwater resources and the risks of saline intrusion under current and future climates (TACTIC WP5).
- Analyse the effectiveness of selected adaptation strategies to mitigate the impacts of climate change (TACTIC WP6).

This report describes the work undertaken by the British Geological Survey (BGS/UKRI) as a part of TACTIC WP4 to calculate groundwater recharge at selected locations within the Permo-Triassic sansdstone aquifer. WP4 is divided into seven tasks that cover the following activities: Review of tools and methods and identification of data requirements (Task 4.1), identification of principal aquifers and their characteristics aided by satellite data (Task 4.2), recharge estimation and its evolution under climate change scenarios in the principal aquifers (Task 4.3), analysis of long-term piezometric time series to evaluate aquifer vulnerability to climate change (Task 4.4), assessment of subsidence in aquifer systems using DInSAR satellite data (Task 4.5),

development of a satellite based net precipitation and recharge map at the pan-European scale (Task 4.6), and tool descriptions and guidelines (Task 4.7).

The work presented here is related to Task 4.3 that aims at the estimation of recharge under current and future climates. This is undertaken using multiple tools selected from the TACTIC toolbox that has been developed undert WP2 of the TACTIC project. The toolbox is a collection of groundwater models, scripts, spreadsheets that serves all the activities identified in TACTIC workpackages. Here we use the lumped groundwater model AquiMod (Mackay et al., 2014a and Mackay et al., 2014b) and the Transfer Function-Noise Model Metran (Zaadnoordijk et al., 2019) with main challenge to calibrate these models to reproduce the behaviour of the observed groundwater level time series. The calibrated models are then used to calculate historical and future recharge values. In addition to these two models, we apply the UK national scale recharge model (Mansour et al., 2018) to validate the calculated recharge values and also to address the uncertainty associated with the calculation of these values.

3 PILOT AREA

3.1 Site description and data

3.1.1 Index boreholes in the Carboniferous Limestone and Devonian sandstone aquifers in the UK

The Carboniferous Limestone aquifer in England and Wales include a wide variety of rock types, such as mudstones, siltstones and sandstones in addition to the limestones. The latter are fractured and well developed as aquifers in the Peak District of Derbyshire, the Mendip Hills, North and South Wales, and northwest Yorkshire (Allen et al., 1997). Where it is a major aquifer, the Carboniferous Limestone aquifer exhibit 'karstic' hydrogeological behaviour.

The Devonian sediments of south Wales and the Welsh borderlands are continental deposits known as the Old Red Sandstone facies (Robins and Davis, 2015). The sediments are divided into the Lower Old Red Sandstone and Upper Old Red Sandstone and there is a major unconformity between them.

In Scotland, the Devonian sandstones in Fife and eastern Scotland are one of the most productive bedrock aquifers in Scotland (Macdonald et al., 2005). The Carboniferous sedimentary rocks have been extensively mined for coal and are largely found in the Midland Valley, with minor outcrops in southern Scotland (O Dochartaigh et al., 2015).

Table 1 shows a list of boreholes located in the Carboniferous Limestone aquifer and to lumped groundwater models are built. These models are used to estimate the historical and future recharge values at these boreholes.

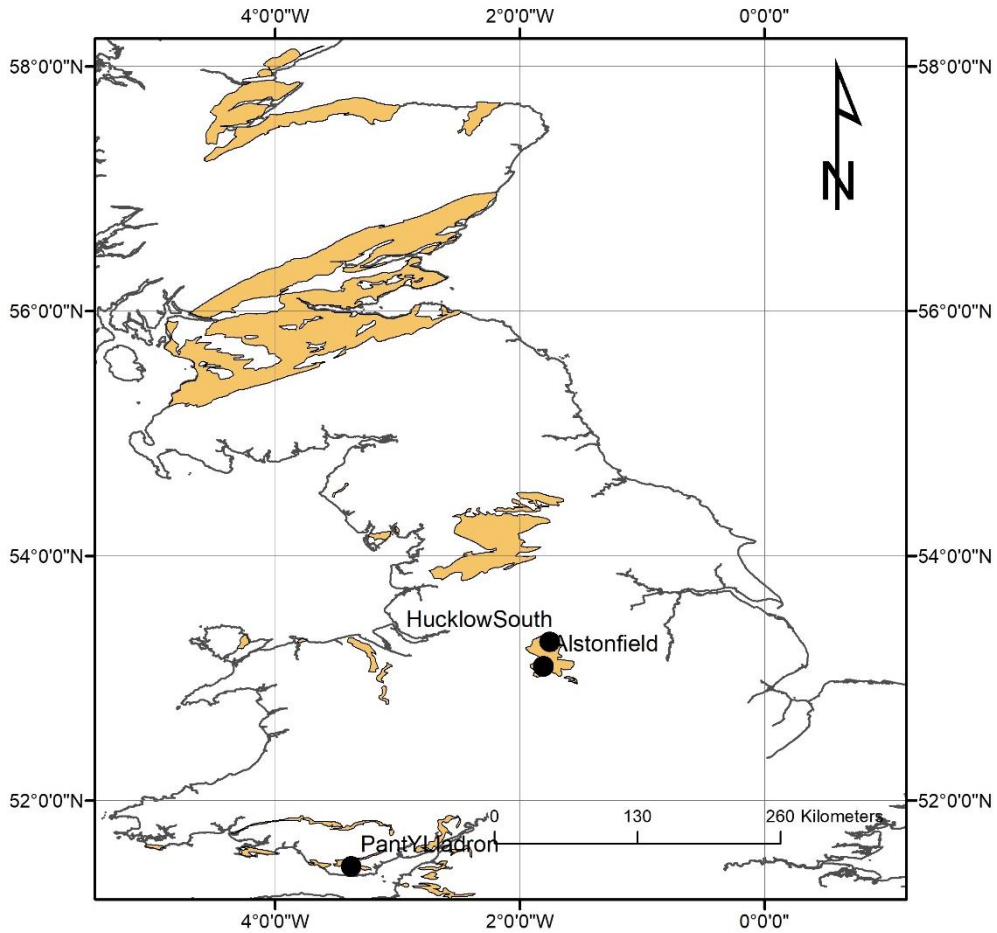


Figure 1. Extent of the Devonian sandstone / Carboniferous Limestone aquifer and borehole locations.

Table 1. Description of observation boreholes

Borehole name	**Location**	**GWLs record**	**Hydrogeological response**
Hucklow South	North of England	1969-2012	The hydrograph has more than one peak in a year due to response to rainfall events.
Alstonefield	Northwest of England	1974-current	The hydrograph is very responsive to seasonal recharge. It has a rapid and peaky response to individual rainfall events through the winter.
Pant Y Lladron	South of Wales	1996-current	The hydrograph shows an annual sinusoidal pattern with significant yearly fluctuations of approximately 20 metres.

3.1.2 Topography

The Devonian/ Carboniferous Limestone aquifers discussed in this report cover different parts across the United Kingdom. Figure 2 shows the ground elevations as obtained from a digital terrain map (Nextmap, 2000). It is clear that the outcrops of the aquifers cover lowlands as well as hills reaching approximately 600 m above sea level. Infiltration recharge drives the groundwater to discharge areas where it appears in the form of springs at the periphery of the hills. Significant quantities of spring flows are used for public water supplies.

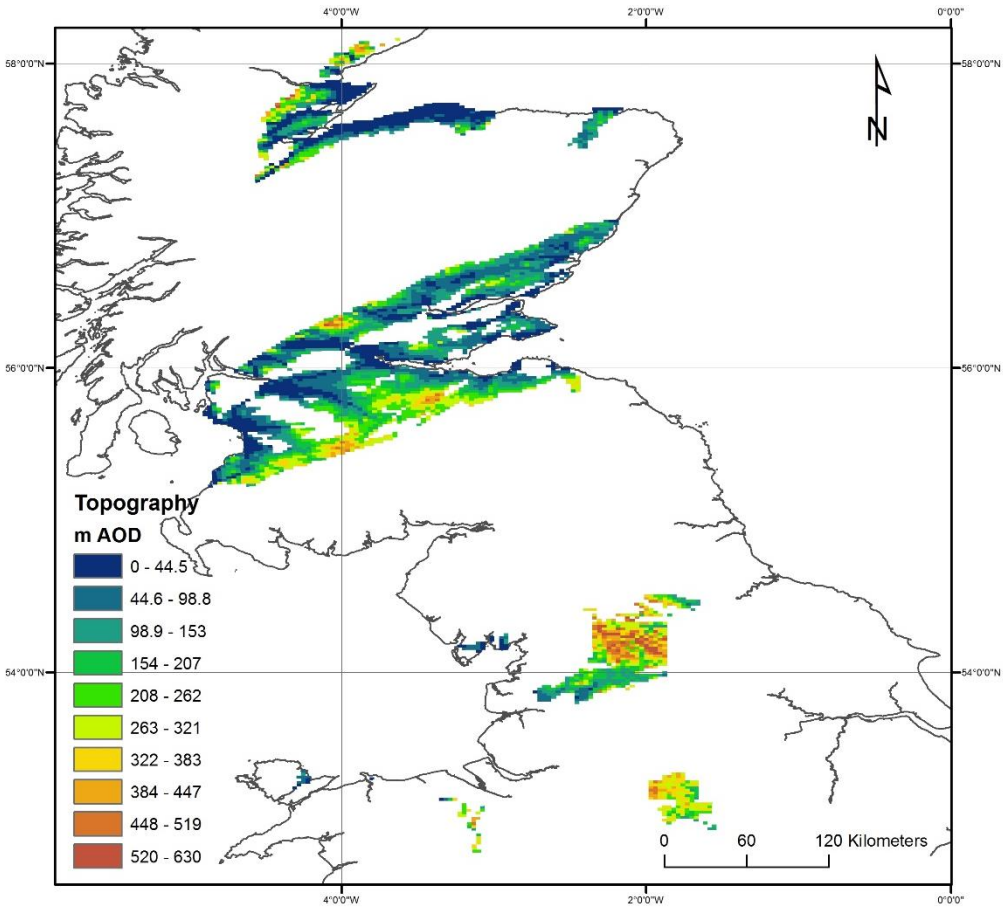


Figure 2. Topography map over the Devonian sandstone / Carboniferous Limestone formation

3.1.3 Land use

The dominant landuse over the aquifer outcrop is mainly arable and improved grassland; however, heath is the majority landuse over the hills especially in north of England. The outcrop incorporates a number of urban and industrial areas including Glasgow (Figure 3). Figure 3 shows the spatial distribution of landuse classes over the Permo-Triassic outcrop (Bibby, 2009).

Landuse data can be extracted from this map at the selected boreholes to specify the model parameters that control evapo-transpiration, which is an important component of the total water balance produced by the applied models. Specific information about the landuse types at the selected boreholes are listed in Table 2.

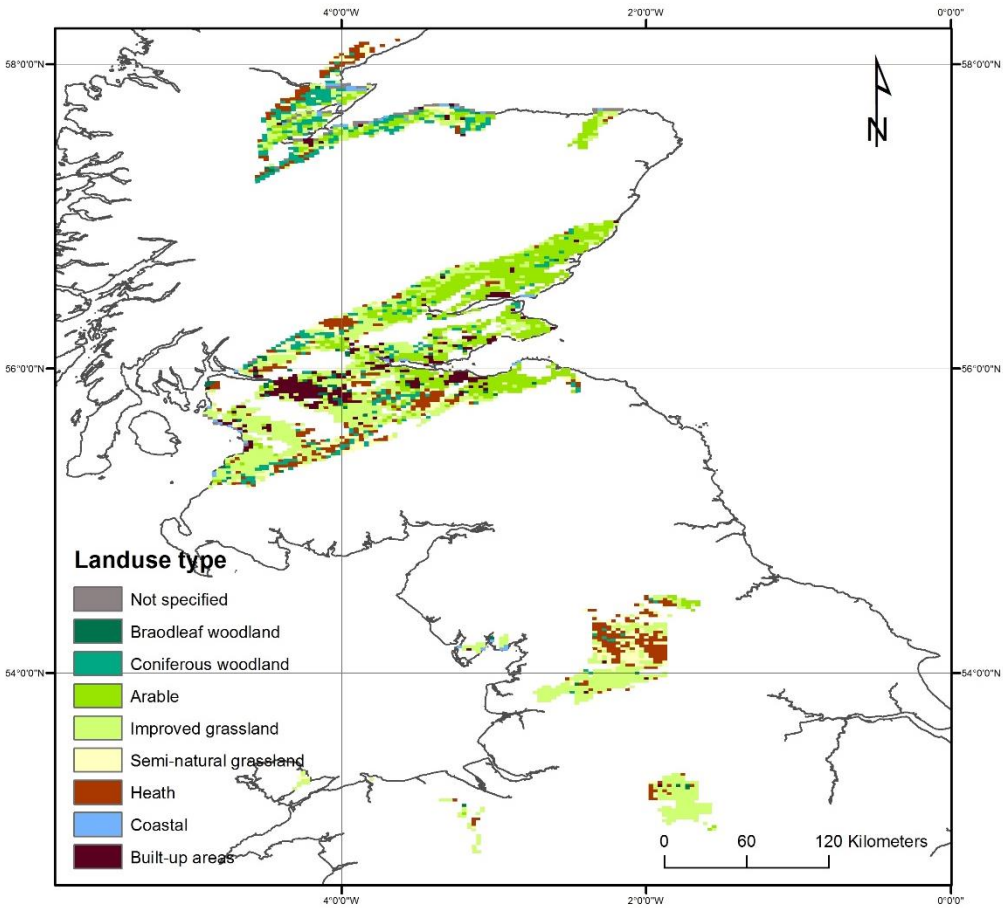


Figure 3. Map of land use over the Devonian sandstone / Carboniferous Limestone formation

3.1.4 Rainfall

Daily rainfall raster data (1 × 1 km) were obtained from the Centre for Ecology and Hydrology (CEH) and were used to retrieve the daily rainfall values at the grid nodes pertain to the Devonian and Carboniferous Limestone aquifers. The long-term average (LTA) rainfall across the outcrop of these aquifers is approximately 1050 mm year^{-1} (2.87 mm day^{-1}); however, high rainfall values more than above 1825 mm year^{-1} (5 mm day^{-1}) are observed in the areas in both north of England and Scotland (Figure 4).

Spatially distributed rainfall data are available at daily time steps starting from 1961 to 2016 (CEH). While the size of this time step is coarse to represent storm events for hydrological analysis, it is fine enough to calculate recharge values to drive groundwater models. These data are, therefore, used to drive the lumped models. Table 2 presents specific information about the rainfall values at the selected Carboniferous Limestone boreholes.

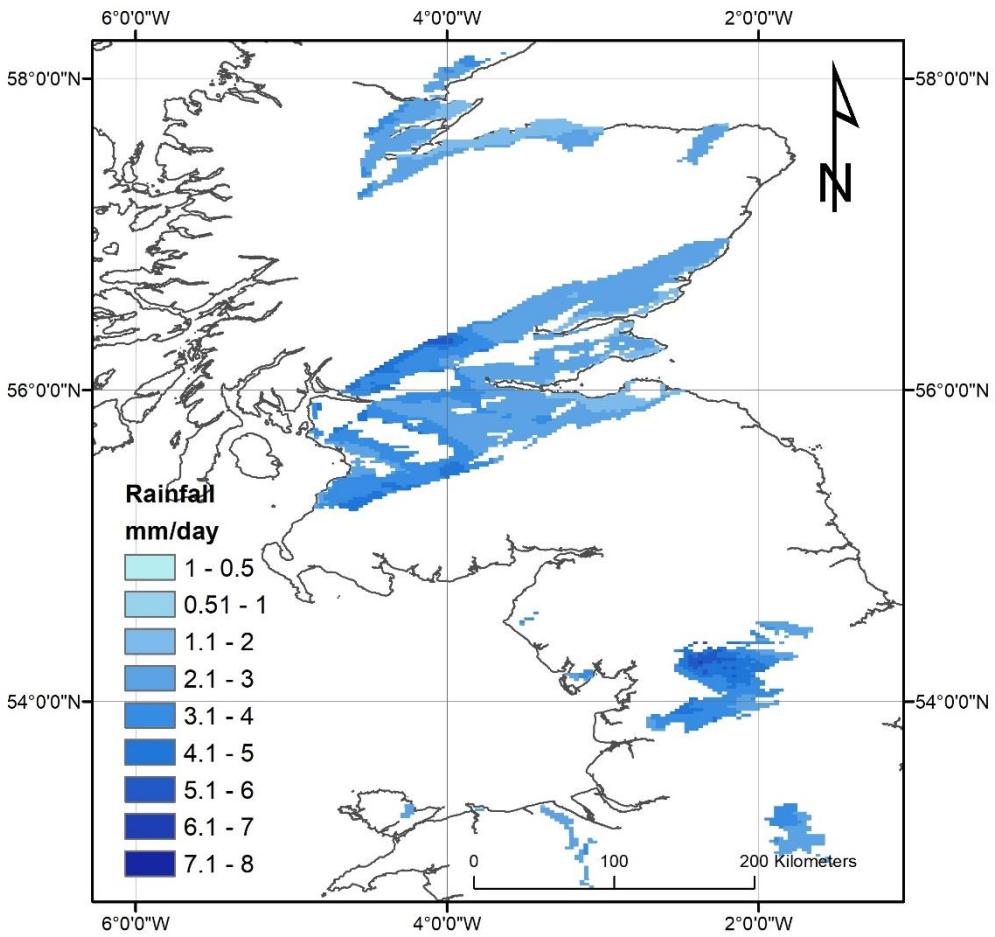


Figure 4. Spatial distribution of rainfall in the Devonian sandstone / Carboniferous Limestone

3.1.5 Potential evaporation

The monthly potential evapotranspiration (PE) raster datasets (40 × 40 km) were gathered from a Met Office Rainfall and Evaporation Calculation System (MORECS) in the Met Office of the UK (Hough and Jones 1997). Figure 5 shows the distributed long-term average potential evaporation data. Highest potential evaporation rates of approximately 686 mm year^{-1} (1.88 mm day^{-1}) are observed to the west of the aquifer outcrop. Lowest potential evaporation rates of approximately 430 mm year^{-1} (1.18 mm day^{-1}) are observed to the north of the aquifer (Figure 5).The average potential evaporation rates over the whole of the Devonian and Carboniferous aquifers is approximately 528 mm year^{-1} (1.45 mm day^{-1}). Table 2 presents specific information about the PE records at the selected boreholes in these aquifers.

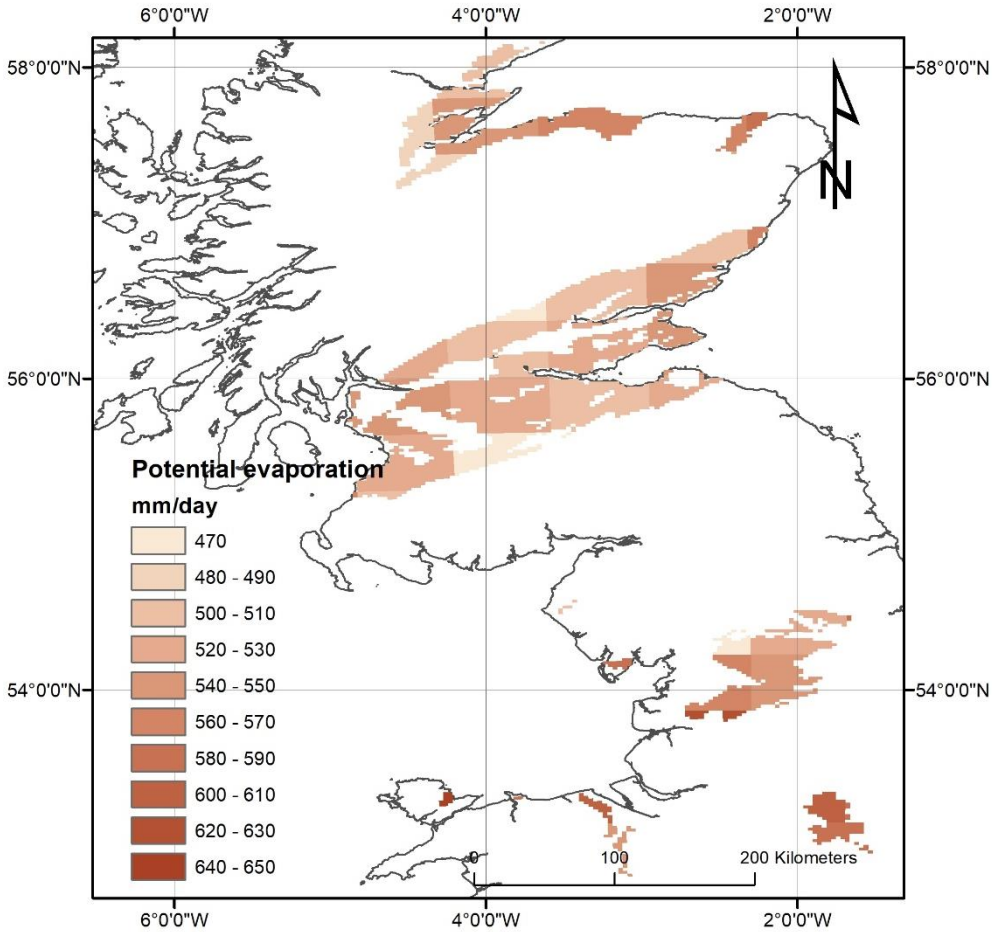


Figure 5. Spatial distribution of potential evaporation in the Devonian sandstone / Carboniferous Limestone

Table 2. Landuse, rainfall and evapotranspiration information for the Permo-Triassic

Borehole name	Dominant landuse	Av. Rainfall (mm/day)	Rainfall record	Av. PE (mm/day)	PE record
Hucklow South	Improved grassland	2.64	1961-current	1.31	1961-current
Alstonefield	Improved grassland	2.84	1961-current	1.61	1961-current
Pant Y Lladron	Improved grassland	3.12	1961-current	1.78	1961-current

3.1.6 Hydrogeology

The Carboniferous Limestone has very low values of porosity and permeability. Analysis on core from north-east England shows porosity values of 0.2% to 5.9% and a median hydraulic conductivity value of 3×10-6 m/d (Nirex, 1993). Secondary network of solution-enlarged fractures (commonly termed conduits) is the main contributor to the aquifer permeability. An important observation in this aquifer is that the conduit networks are continuously changing, which makes the karst systems a dynamic one. In general, karst systems will tend to evolve downwards, with newly developed lower conduit networks and drying up the upper networks.

In the Devonian sandstones in Fife and eastern Scotland, there is considerable variation in porosity and hydraulic conductivity with depth in the aquifer. Geophysical logging shows that fracture flow is dominant even where porosity high porosity exits. Mean porosity from four formations is approximately 20% and analysis of pumping tests from five boreholes show transmissivity values varying between 200 and 800 m^2 day^{-1} (Macdonald et al., 2005). No lumped models are discussed in this study for boreholes located in this aquifer.

The productivity of Carboniferous sedimentary rocks in Scotland which depends on the nature of natural fracturing as well as on the extent and nature of mining impacts. Mine voids can artificially and greatly increase aquifer transmissivity. Aquifer storage can also be locally increased. The productivity of Carboniferous aquifers subject to extensive coal mining is reflected by the higher yield of boreholes drilled through these mines.

The Old Red Sandstone in Wales is approximately 2 km thick in places, but has no significant groundwater storage and transport; however, this aquifer is still arguably the most important aquifer in Wales. The principal controls on permeability and transmissivity arise from lithology changes, degree of induration/cementation, and extent/depth of fracturing along bedding planes. Transmissivity values obtained from pumping test analysis reach 350 m^2 day^{-1}, with a mean of 51 m^2 day^{-1}.

3.1.7 Groundwater levels

Depending on the investigated location, the aquifer can be under confined or unconfined conditions. At Huclow South, no superficial deposits are mapped on the ground surface, but clay and stones were encountered when drilling. The water is unconfined with a large seasonal range of about 25 m. At Alstonefield the water level hydrograph represents an open groundwater system. The water level in the borehole is relatively deep and reflects a regional water level controlled by drainage in the incised valley of the River Dove to the south of the borehole.

These time series of groundwater levels are used in this study to characterise the aquifer properties and to estimate the infiltration recharge values for water resources management. The boreholes are selected so that they are not significantly impacted by the presence of nearby surface features.

3.2 Climate change challenge

The British Geological Survey (BGS) with the support of the Environment Agency (EA) have undertaken a study to investigate the impact of climate change on groundwater resources using the distributed recharge model ZOODRM (Mansour and Hughes, 2018). Potential recharge values for Great Britain (England, Scotland and Wales) are produced using rainfall and potential evaporation data from the Future Flows Climate datasets (11 ensembles of the HadCM3 Regional Climate Model or RCM). This study has shown that generally the recharge season appears to be forecast to become shorter, but with greater amount of recharge "squeezed" into fewer months. This conclusion is aligned with the European Environment Agency map that describes the expected climate change across the different areas in Europe as shown in Figure 6.

The shortening of recharge season indicates that aquifers may become more vulnerable to droughts if rainfall fails in one or two months rather than a prolonged dry winter as can occur now. At the very least, water management measures have to be put in place to account for periods when recharge volumes reduce. On the other hand, the increased recharge signal could result in flashier groundwater level response and potentially leading to more flooding.

The main climate challenge for water resources managers and stakeholders is to assess the risk of future flooding and drought events. This requires detailed assessment of the variation of resources at regional and local scales rather than national or continental scales.

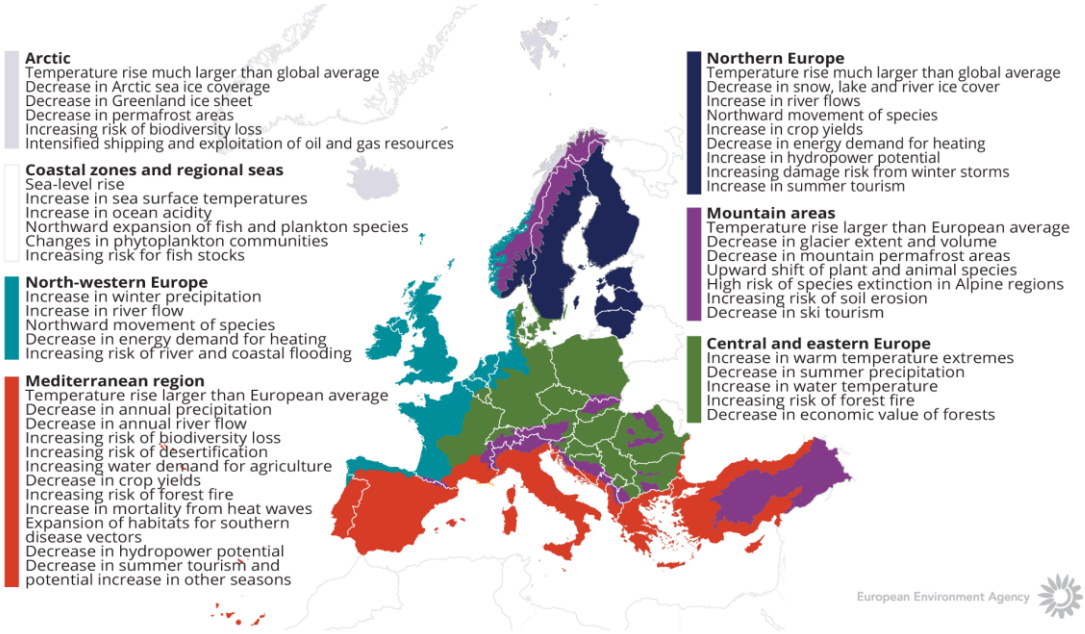


Figure 6. How is climate expected to change in Europe. The European Environment Agency map

4 METHODOLOGY

4.1 Methodology and climate data

4.1.1 AquiMod

AquiMod is a lumped parameter computer model that has been developed to simulate groundwater level time series at observational boreholes (Mackay et al., 2014a). It is based on hydrological algorithms that simulate the movement of groundwater within the soil zone, the unsaturated zone, and the saturated zone. The lumped models neglect complexities included in distributed groundwater models but maintain some of the fundamental physical principles that can be related to the conceptual understanding of the groundwater system (Mackay et al., 2014b).

The primary aim of AquiMod is to capture the behaviour of a groundwater system through the analysis of the available groundwater level time series. Once calibrated the model can be run in predictive mode and be used to fill in gaps in historical groundwater level time series and to calculate future groundwater levels. In addition to groundwater levels, it also provides predictions of historical and future recharge values and groundwater discharges.

The mathematical equations that are used to simulate the movement of groundwater flows within the three modules are detailed in Appendix A. The model uses rainfall and potential evaporation time series as forcing data. These are interpreted by the soil module representing the soil zone. The soil module calculates the rainfall infiltration and pass it to the unsaturated zone module. This module delays the arrival of the infiltrating water to the saturated zone module. The latter calculates the variations of groundwater heads and flows accordingly.

The model is calibrated using a Monte Carlo approach. It compares the simulated and observed groundwater level fluctuations and calculates a goodness of fit. The AquiMod version used in this work employs the Root Square Mean Error (RMSE) or the Nash Sutcliffe (NSE) performance measures to assess the performance of the model. The user sets a threshold value to accept all the models that perform better than the specified threshold. The possibility of producing many models that are all equally acceptable, allows the user to interpret the results from all these models and calculate uncertainty.

The recharge values calculated form AquiMod are those that reach the aquifer system and drive the groundwater levels. Thus, it is assumed that these are the actual recharge values as defined by the guidance report prepared by TACTIC project

4.1.2 Metran

Metran applies a transfer function-noise model to simulate the fluctuation of groundwater heads with precipitation and evaporation as independent variables (Zaadnoordijk et al., 2019). The modelling approach consists mainly of two impulse functions and a noise model. The first impulse function is used for convolution with the precipitation to yield the precipitation contribution to the piezometric head. The second is for evaporation which is either a separately estimated function, or a factor times the function used for precipitation. The noise model is a

stochastic noise process described by a first-order autoregressive model with one parameter and zero mean white noise. Further information about the model is given in Appendix B with the model setup shown in the Figure B1.

Metran allows the addition of other processes affecting the behaviour of the groundwater heads, for example pumping or the presence of surface features such as rivers. The contributions from these processes are added to the deterministic part of the model.

Metran has been designed to work with explanatory series that have a daily time step. However, it has been adapted so that other time step lengths can be applied. However, the explanatory variables must still have a constant frequency.

The model is calibrated automatically; however, the model uses two binary parameters, Regimeok and Modok, to judge a resulting time series model. Regimeok cross-examines the explained variance R2 (> 0.3), the absolute correlation between deterministic component and residuals (< 0.2), and the null hypothesis of non-correlated innovations (p value > 0.01). If all these criteria are satisfied, Regimeok returns a value of 1 indicating highest quality. Modok also cross-examines the explained variance R2 (> 0.1) and the absolute correlation between deterministic component and residuals (< 0.3) as well as the decay rate parameter (> 0.002) and if all these criteria are satisfied, it is given a value of 1. If Modok = 1 and Regimeok = 0, the model is still considered acceptable. If both these parameters are 0, the model quality is insufficient and the model is rejected.

Metran's time series model is linear and the model creation fails when the system is strongly nonlinear. It is also limited to the response function being appropriate for the simulated groundwater system. Metran uses a gradient search method in the parameter space, so it can be sensitive to initial parameter values in finding an optimal solution.

The model calculates an evaporation factor f that gives the importance of evapotranspiration compared to precipitation. It is possible to use this factor to calculate the recharge values as shown by Equation B2 in appendix B. However, it must be noted that the use of Equation B2 is based on too many assumptions that are easily violated. Because of this, the equations should be applied only to long-term averages using only models of the highest quality.

Following the definitions used in the TACTIC project, this recharge quantity corresponds to the effective precipitation. It is equal to the potential recharge when the surface runoff is negligible. This in turn is equal to the actual recharge at the groundwater table if there is also no storage change or interflow.

4.1.3 The distributed recharge model ZOODRM applied at the UK scale

A distributed recharge model, ZOODRM, has been developed by the British Geological Survey to calculate recharge values required to drive groundwater flow simulators. This recharge model allows grid nesting to increase the resolution over selected area and is called therefore the zooming object-oriented distributed recharge model (ZOODRM) (Mansour and Hughes, 2004). The model can implement a number of recharge calculation methods that are suitable for

temperate climates, semi-arid climates, or for urban areas. One of the methods that is implemented is the recharge calculation method used by AquiMod and detailed in Appendix A1.

ZOODRM uses a Cartesian grid to discretise the study area. It reads daily rainfall and potential evaporation data in time series or gridded format and calculates the recharge and overland flow at a grid node using a runoff coefficient as detailed in appendix A1. However, since this is a spatially distributed model, it reads a digital terrain model and calculates the topographical gradients between the grid nodes. It then uses the steepest gradient to route the calculated surface water downstream until a surface feature, such as a river or a pond, is reached. While the connections between the grid nodes based on the topographical gradients define the water paths along which surface water moves, major rivers are also user-defined in the model. This allows the simulation of river water accretion on a daily basis and the production of surface flow hydrograph. The model is then calibrated by matching the simulated river flows at selected gauging stations to the observed flows, by varying the values of the runoff coefficients.

The procedure used to calibrate the model involves dividing the study area into a number of zones and then to specify runoff values for each one. It is possible to vary the runoff coefficient values on a seasonal basis by using different runoff values for the different months of the year.

The recharge model ZOODRM calculates rainfall infiltration after accounting for evapo-transpiration and soil storage. The simulated infiltration may not reach the aquifer system as it may travel laterally within the soil and discharge into surface water features away from the infiltration location. The simulated infiltration is therefore considered, as potential recharge according to the definitions of recharge processes provided by the guidance report prepared by TACTIC project.

Climate data

The TACTIC standard scenarios are developed based on the ISIMIP (Inter Sectoral Impact Model Intercomparison Project, see www.isimip.org) datasets. The resolution of the data is 0.5°x0.5°C global grid and at daily time steps. As part of ISIMIP, much effort has been made to standardise the climate data (e.g. bias correction). Data selection and preparation included the following steps:

1. Fifteen combinations of RCPs and GCMs from the ISIMIP data set where selected. RCPs are the Representative Concentration Pathways determining the development in greenhouse gas concentrations, while GCMs are the Global Circulation Models used to simulate the future climate at the global scale. Three RCPs (RCP4.5, RCP6.0, RCP8.5) were combined with five GCMs (noresm1-m, miroc-esm-chem, ipsl-cm5a-lr, hadgem2-es, gfdl-esm2m).
2. A reference period was selected between 1981 – 2010 and an annual mean temperature was calculated for the reference period.
3. For each combination of RCP-GCM, 30-years moving average of the annual mean temperature where calculated and two time slices identified in which the global annual mean temperature had increased by +1 and +3 degree compared to the reference period, respectively. Hence, the selection of the future periods was made to honour a

specific temperature increase instead of using a fixed time-slice. This means that the temperature changes are the same for all scenarios, while the period in which this occur varies between the scenarios.

4. To represent conditions of low/high precipitation, the RCP-GCM combinations with the second lowest and second highest precipitation were selected among the 15 combinations for the +1 and +3 degree scenario. This selection was made on a pilot-by-pilot basis to accommodate that the different scenarios have different impact on the various parts of Europe. The scenarios showing the lowest/highest precipitation were avoided, as these endmembers often reflects outliers.
5. Delta change values were calculated on a monthly basis for the four selected scenarios, based on the climate data from the reference period and the selected future period. The delta change values express the changes between the current and future climates, either as a relative factor (precipitation and evapotranspiration) or by an additive factor (temperature).
6. Delta change factors were applied to local climate data by which the local particularities are reflected also for future conditions. These monthly values (one set of rainfall and PE for each warming scenario) are used to drive the groundwater models presented in this report.

For the analysis in the present pilot the following RCP-GCM combinations were employed:

Table 3. Combinations of RCPs-GCMs used to assess future climate

		RCP	GCM
1-degree	"Dry"	rcp6p0	noresm1-m
	"Wet"	rcp4p5	miroc-esm-chem
3-degree	"Dry"	rcp4p5	hadgem2-es
	"Wet"	rcp8p5	miroc-esm-chem

4.2 Model set-up

4.2.1 AquiMod

The boreholes located in the Carboniferous Limestone aquifer are listed in Table 1. Aquimod model setup relies mainly on two input files. The first input file "Input.txt" is a control file where the module types and model structure are defined. AquiMod is executed first under a calibration mode where a range of parameter values of the different selected modules are given in corresponding text files and a Monte Carlo approach is used to select the parameter values that yield best model performance. "Input.txt" also controls the mode under which AquiMod is executed, the number of Monte Carlo runs to perform, the number of models to keep with an acceptable performance, and the number of runs to execute in evaluation mode.

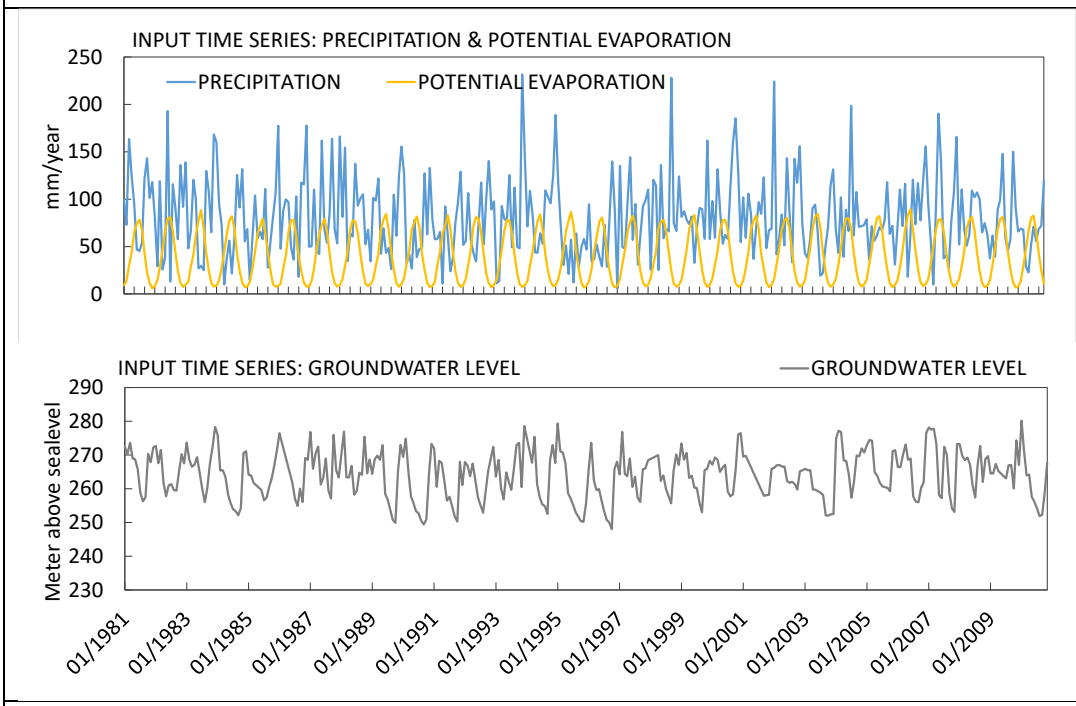
The second file AquiMod uses is called "observations.dat". This file holds the forcing data mainly the potential evaporation and rainfall. However, it is also possible to include the anthropogenic impact on groundwater levels by including a time series of pumping data in this file. None of the boreholes studied here includes pumping data. The observed groundwater levels that are used

for model calibration are also given in this file. The data are provided to the model on a daily basis, and this forces AquiMod to run using a time step length of one day. Table 4 shows daily time series of rainfall and potential evaporation values (mm/month) as well as the fluctuations of water table at the different boreholes.

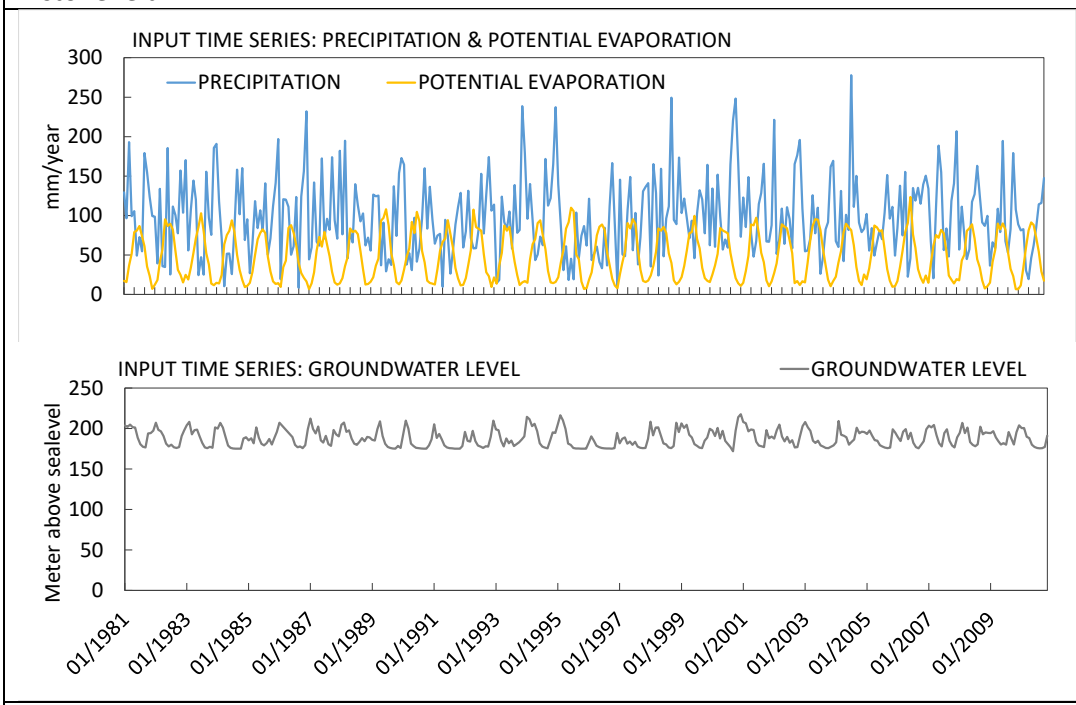
All AquiMod models built for the boreholes in Table 1 use the FAO Drainage and Irrigation Paper 56 (FAO, 1988) method in the soil module, and employ the two-parameter Weibull probability density function to control the movement of infiltrated water in the unsaturated zone (Appendix A1). However, the groundwater module structures vary between the different boreholes. The best groundwater module structure is found by trial and error during the calibration process. The simplest structure, one layer with one discharge feature, is selected first and then the complexity of the module structure is increased gradually to see if the model performance improves. The structure with best model performance is selected to undertake the recharge calculations. The structures selected for these boreholes are mainly of one layer or three-layered systems.

Table 4 Figures showing time series of daily rainfall and potential evaporation values (mm/month) as well as the fluctuations of water table at the different boreholes.

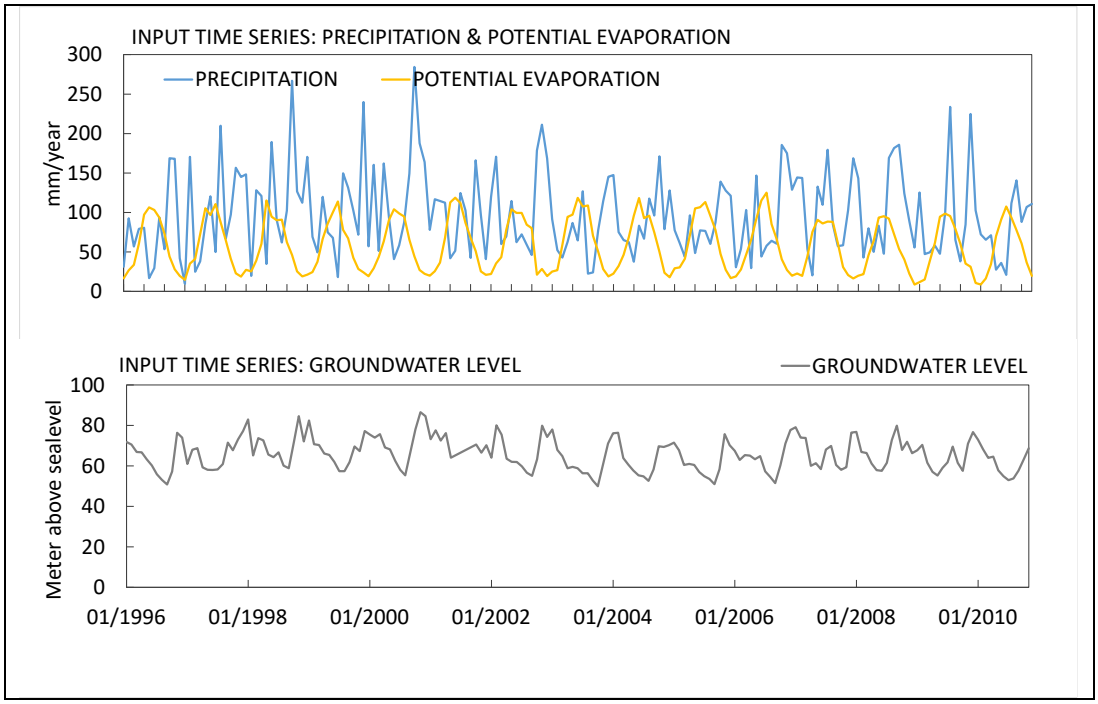
Hucklow South



Alstonefield



Pant Y Lladron



4.2.2 Metran

Metran applies transfer function noise modelling with daily precipitation and evaporation as input and of groundwater levels as output (Zaadnoordijk et al., 2019). The setup is shown in Figure 7. If time series of other influences on the groundwater head are available, these contributions can be added to the deterministic part of the model. An input file that holds the daily information of precipitation, potential evaporation and groundwater levels is prepared for each borehole in Table 1. Plots of these data are shown in Table 4. It must be noted that, while the groundwater levels used in AquiMod and shown in Table 4 have missing values, these have to be provided as complete time series to Metran. To achieve this, a linear interpolation procedure is used to fill in the missing values in the groundwater level time series.. Once executed, it calculates the characteristics of the impulse functions and the corresponding parameters automatically.

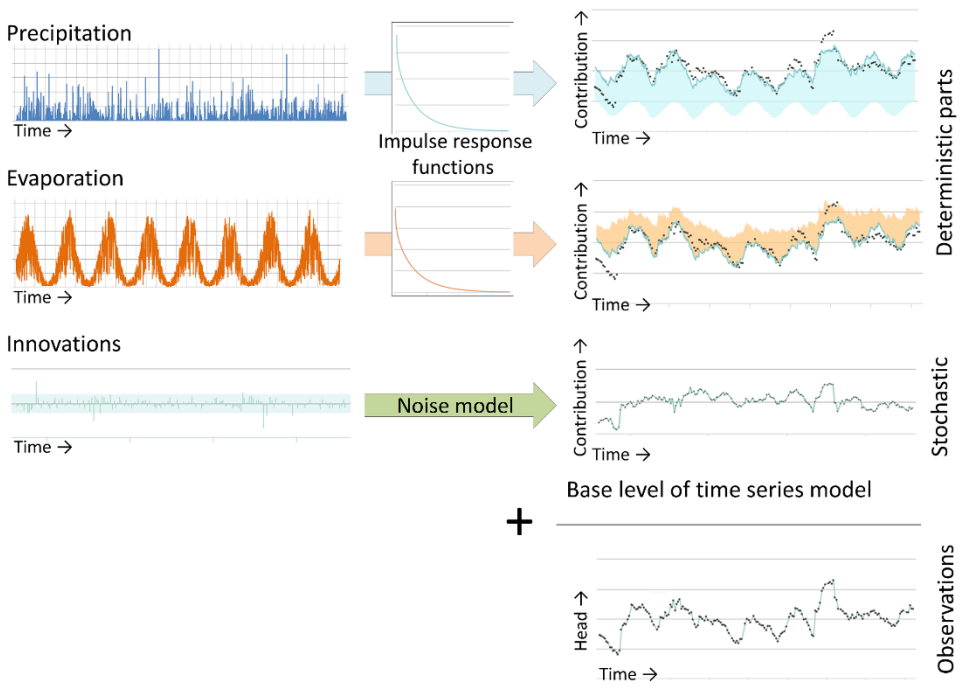


Figure 7 Illustration of METRAN setup

4.2.3 National scale model (ZOODRM)

The distributed recharge model (ZOODRM) is applied at national over the British Mainland (England, Scotland, and Wales) (Figure 8) using a Cartesian grid with 2 km square cells. The model reads a text file that defines the locations of the grid nodes as well as the connections between the nodes. This text file is prepared using a specific tool, called ZETUP (Jackson, 2004), where the extent of the study area is defined using the coordinates of the lower left and upper right corners of a rectangle that covers the modelled area. The spacing between the nodes and the information that dictate the boundary of the irregular shape of the area are also given in this file. This tool also uses a file that contains the locations of the nodes as obtained from a geographical information system tool (GIS) and converts this information into a text file that describes the river extents and characteristics.

The map defining the runoff zones is based on the hydrogeology of the study area. It is produced in gridded *ascii* format using the hydrogeological map available for Great Britain. Additional text files, one for each runoff zone, are also prepared to define the monthly runoff values.

The topographical information is also provided in a gridded *ascii* format for the model to calculate the topographical gradients between the nodes. While a surface water routing procedure that accounts for indirect recharge and surface water storage is available in the model, this is not used in the current application. It is assumed that all the water originated at one grid nodes travel downstream and reaches a discharging feature in one day, which is equal to the length of the time step used.

Landuse data (Section **Error! Reference source not found.**) and soil data that are required to calculate the water capacity at every grid node are also provided to the model using maps in gridded *ascii* format. A set of ten gridded landuse maps are used to give the percentage of landuse type at any given location. The gridded soil map gives the soil type at a selected location. The landuse type and soil type ids are linked to text files that hold the corresponding information such as the soil moisture at saturation, the soil moisture at wilting and the root constants can be obtained.

The driving data are provided to the model as daily gridded rainfall data (Sections **Error! Reference source not found.**) and time series of monthly potential evaporation values as described in (Section **Error! Reference source not found.**). Mansour et al. (2018) provide a full description of the construction of this model together with a more detailed description of the data used. The calculated recharge values are also provided in the published work; however, it must be noted that the historical recharge values shown in this work are simulated over the period from 1981 to 2010 in order to be consistent and comparable with the recharge values calculated by AquiMod and Metran. In addition, in this study, the model has been rerun using the climate change data specifically provided by the TACTIC project to calculate the projected distributed recharge values.

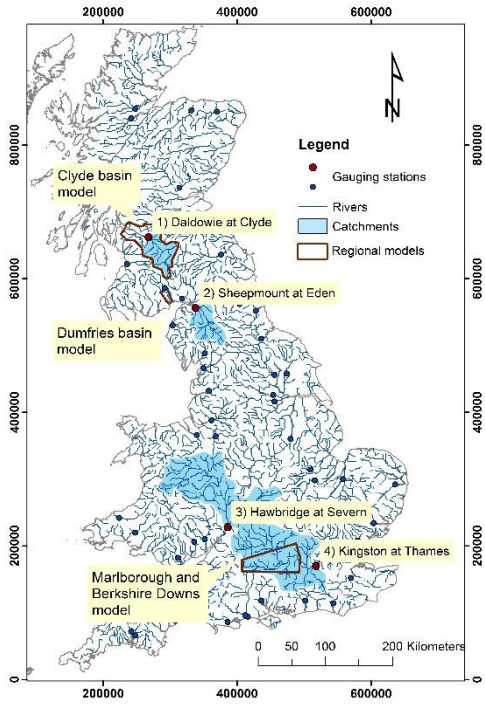


Figure 8. Extent of the UK national scale recharge model in UK national grid reference after Mansour et al. (2018). Figure also shows the locations of the gauging stations downstream of the major rivers used for model calibration.

4.3 Model calibration

4.3.1 Calibration of AquiMod models

The calibration of AquiMod is performed automatically using the Monte Carlo approach. The user populates the files of the selected modules with minimum and maximum parameter values and then the model randomly selects a value from the specified range for any given run. The selection of the minimum and maximum values is physically based depending on the characteristics of the study area. For example, the minimum and maximum values of the root depth in the soil module are set to 15 cm and 60 cm respectively for a study area covered with grass, while these values are set to 120 cm and 200 cm for a woodland area. The storage coefficients bounds of a groundwater module are set to much lower values in a confined aquifer compared to those used for an aquifer under unconfined conditions.

A conceptual hydrogeological understanding must be available before the use of AquiMod, since this is necessary to set the limits of the parameter values for the calibration process. In some cases, it is not possible to obtain a good performing model with the selected values and that necessitates the relaxation of these parameters beyond the limits informed by the conceptual understanding. In such cases, the parameter values must feed back into the conceptual understanding if better performing models are obtained.

AquiMod execution time is relatively small, which allows the calibration of the model using hundreds of thousands of runs in couple of hours. The performance measure used to assess the quality of the simulation is the Nash Sutcliffe Error (Appendix A) that takes a maximum value of unity for a perfect match between the simulated and observed data. The threshold at which models are accepted is set to a value of 0.6. All the models that achieve an NSE higher than 0.6 are included in the analysis but a maximum number of 1000 runs are used if the number of acceptable models is greater than 1000.

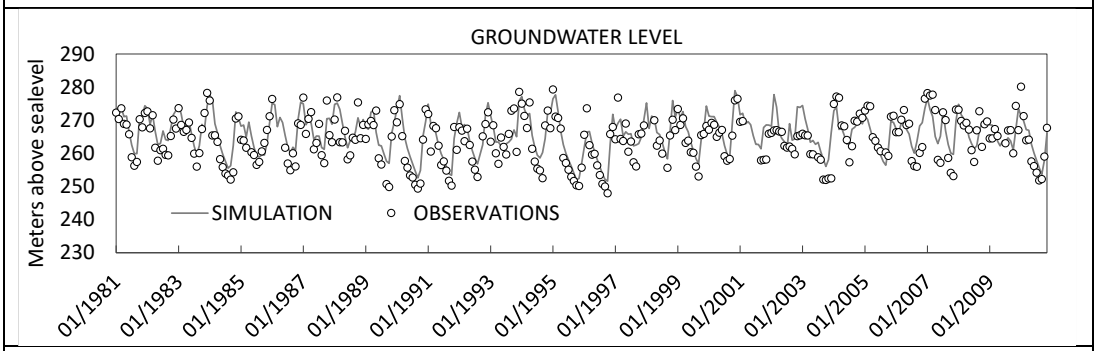
Table 5 shows the best NSE values obtained for the models calibrated at the Devonian sandstone / Carboniferous Limestone boreholes listed in Table 1. It is clear that a good match was achieved between the simulated and observed groundwater levels as illustrated in the plots shown in Table 6. The best performing model is the AquiMod model built at PantYLladron borehole with an NSE value of 0.92. The least performing AquiMod model is that built for Hucklow South borehole with an NSE value of 0.75.

Table 5 Nash Sutcliff Error measure at the Devonian sandstone / Carboniferous Limestone boreholes

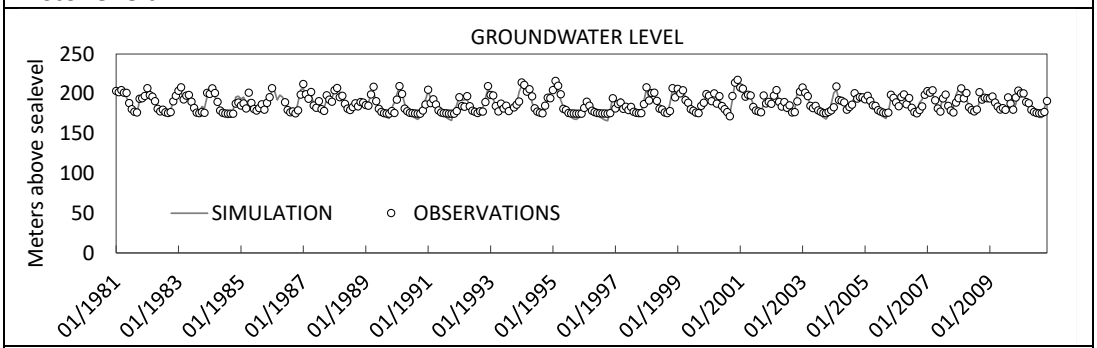
Borehole name	**NSE**
Hucklow South	0.75
Alstonefield	0.89
Pant Y Lladron	0.92

Table 6 Comparison between the simulated and observed groundwater levels at the Devonian sandstone / Carboniferous Limestone observation boreholes.

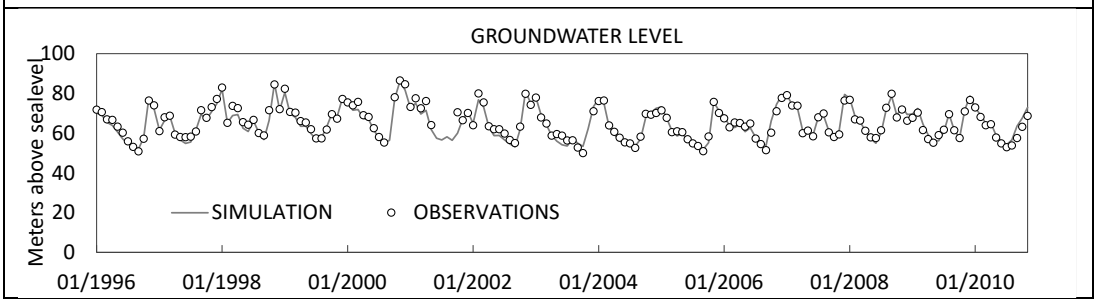
Hucklow South



Alstonefield



Pant Y Lladron



4.3.2 *Calibration of Metran models*

For the standard setup with precipitation and evaporation, there are five parameters that have to be determined during the calibration of the model. Three parameters are related to the precipitation response, the evaporation factor, and the noise model parameter (Appendix B). There are three extra parameters for each additional input series, such as pumping. The parameter optimization of Metran uses a gradient search method in the parameter space to reach a global minimum. As explained in Appendix B, two parameters indicate if Metran succeeded with producing a match between the simulated and observed data. These are called the Regimeok and Modok. When Regimeok is equal to one, the calibration is of highest quality. If Modok is equal to one and Regimeok is equal to zero, the calibration is of acceptable quality. Finally, if both parameters are equal to zero, the calibration quality is insufficient.

Time series of rainfall, potential evaporation and groundwater levels are provided to Metran on a monthly basis. Metran input data must be complete dataset, i.e. without missing data. To overcome this problem that may exist in the groundwater level time series, these data are aggregated to monthly values first and then missing values were filled using linear interpolation. Table 7 shows the performance of Metran across the Carboniferous Limestone boreholes considered in this study. It is clear that according to criteria set above, Metran fails to produce a model at four boreholes but succeeds at the Hucklow South borehole; however, Metran produces acceptably performing models at Alestonefield and Pant_Y_Lladron with the model output showing highest quality is the one found for Alestonefield with R^2 value of 0.81.

Table 7 Performance of Metran across the selected Devonian sandstone / Carboniferous Limestone boreholes.

Borehole name	Metran performance parameter Modok	Metran performance parameter Regimeok	Overall quality	R2	RMSE
Hucklow South	0	0	Insufficient	0.55	4.34
Alstonefield	1	0	Acceptable	0.81	4.39
Pant Y Lladron	1	0	Acceptable	0.66	5.14

4.3.3 *Calibration of the UK national scale model using ZOODRM*

Model calibration of the national scale recharge model was based on the comparison of the simulated long-term average overland flows to the observed ones (Mansour et al., 2018) recorded at gauging stations of selected major rivers (Figure 8). However, additional checks were also undertaken to assess the performance of the model. These include checking the match between the seasonal overland flow volumes at four boreholes, shown in red in Figure 8, checking the calculated recharge volumes with those calculated by other tools over selected catchment areas, and checking the temporal fluctuations of soil moisture deficit with those

calculated by other tools. Figure 9 shows a Q plot for the simulated vs observed long term average runoff values at the 56 gauging stations shown in Figure 8. The solid line shows the one to one match and the dotted line shows the linear relationship between the two datasets.

It must be noted that while this model uses the same recharge calculation methods used by AquiMod, these two models are calibrated using different datasets, with AquiMod using the groundwater levels and the distributed recharge model using the overland flows.

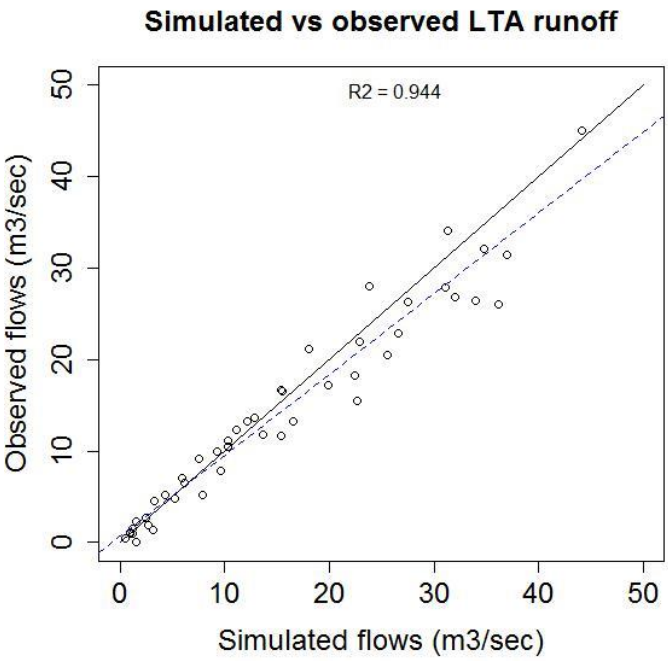


Figure 9 Q plot for the simulated vs observed long term average runoff values at the 56 gauging stations shown in Figure 8 after Mansour et al. (2018)

5 RESULTS AND CONCLUSIONS

5.1 Historical recharge values

Table 8 shows the time series of the historical recharge values calculated using the AquiMod model at the Carboniferous Limestone boreholes listed in Table 1. The plots in this table also show the 10th percentile, the mean, and the 90th percentile of recharge values calculated from the time series.

As mentioned in Appendix B, the formulas used by Metran are based on assumptions that can be violated and it is better to use the infiltration coefficient f_c with the long-term average values of rainfall and potential evaporation to calculate long-term average values of recharge and using only models of the highest quality. Time series of recharge values are not therefore produced, from the analysis undertaken using Metran. The long-term average recharge values calculated using Metran are shown in Table 9.

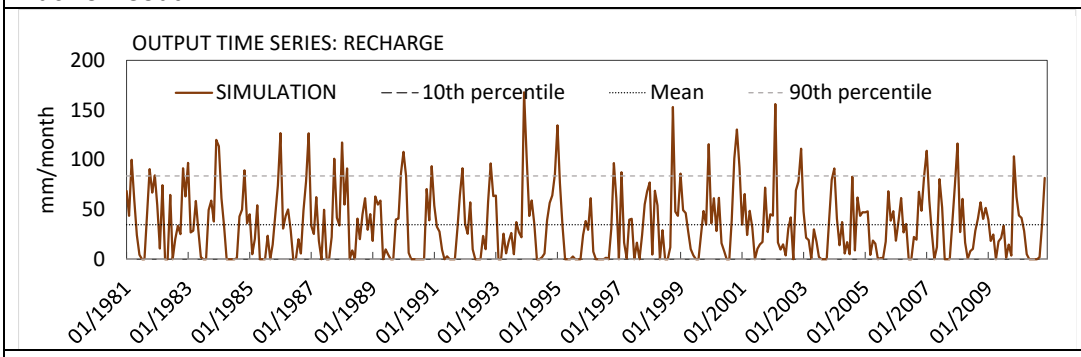
One of the benefits of running AquiMod in Monte Carlo mode is the possibility of producing many models with acceptable performance. Consequently, the recharge values estimated from these models are all equally likely. This provides us with a range of recharge values at each borehole that reflects the uncertainty of the optimised hydraulic parameter values. In the current study, the long-term average recharge values are calculated from up to 1000 acceptable models if they exist at each borehole; otherwise, all the acceptable models are used. The mean, 25th and 75th percentiles are then calculated from these long-term recharge values and displayed in Figure 10. It is clear that the differences between the 75th and 25th percentile values is negligible at Hucklow South borehole but more noticeable at the other two boreholes. At PantYLladron, the difference between the 25th and the 75th percentile values is approximately 8 mm/month (27%) and at Alestonefield the difference is approximately 5.7 mm/month (18.5%).

In addition to the recharge values calculated using AquiMod, Figure 10 shows the recharge values calculated using Metran and the distributed national scale model at these boreholes. It is clear that there is a good agreement between the AquiMod calculated recharge values and those calculated using the distributed national scale model at PantYLladron; however, there are significant differences at Hucklow South and Alestonefield with the national scale model producing significantly higher values at these boreholes. It must be noted that the recharge values calculated by these two models are of different types. The distributed recharge model calculates potential recharge and AquiMod calculates actual recharge.

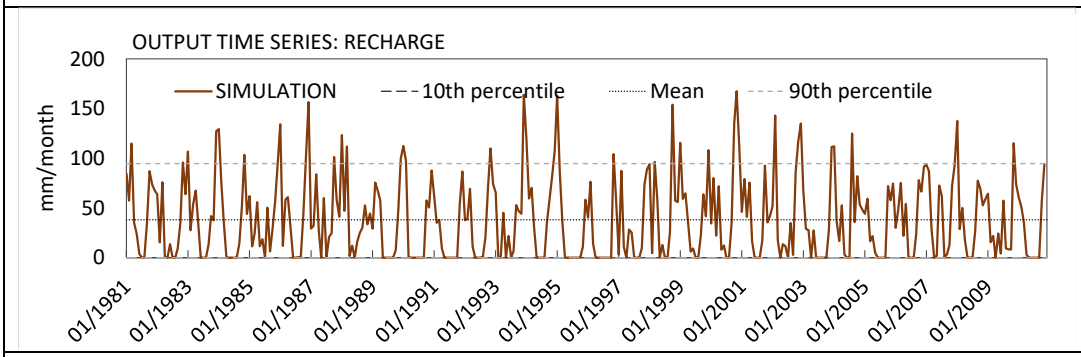
Metran produces significantly different values from AquiMod at all three boreholes. While the recharge value produced by Metran at Hucklow South is shown in Figure 10, it must be treated with caution ass Metran reported badly performing model at this borehole. Metran estimates an upper and a lower value for the infiltration coefficient f_c. This can be used as an indication of uncertainty associated with the calculated f_c value. These bounds are also shown in Table 9.

Table 8 Time series of recharge values obtained from the best performing AquiMod models at the Devonian sandstone / Carboniferous Limestone boreholes

Hucklow South



Alstonefield



Pant Y Lladron

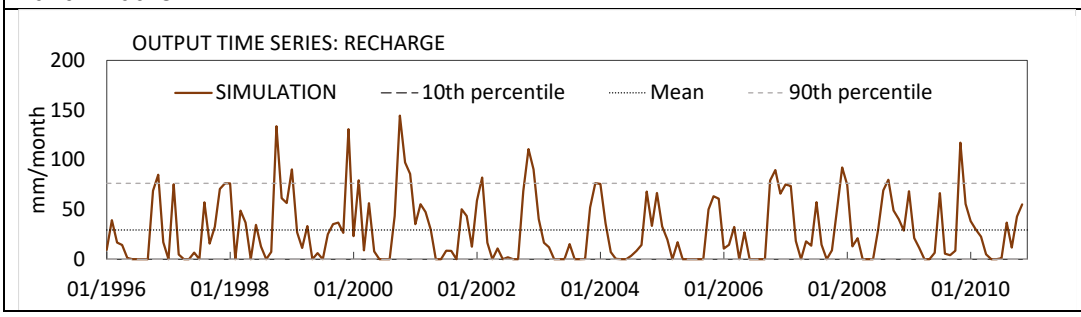


Table 9 Recharge values calculated using the recharge factors estimated by Metran

Borehole name	Average precipitation (mm/month)	Average potential evaporation (mm/month)	Recharge factor	Recharge (mm/month)
Hucklow South	80.63	39.95	1.49 +- 0.56	14.17
Alstonefield	86.47	48.98	1.24 +- 0.24	20.54
Pant Y Lladron	95.12	54.34	0.66 +- 0.203	59.42

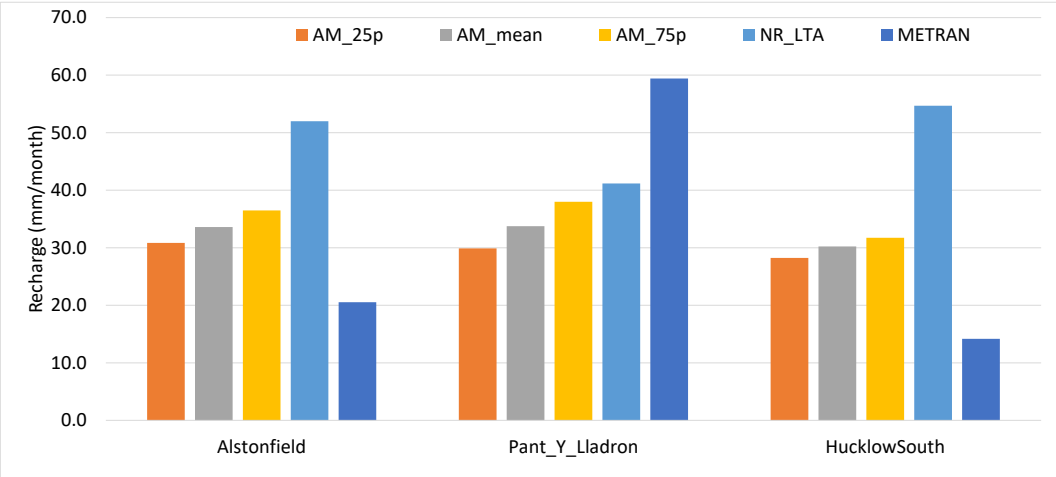


Figure 10 Historical recharge values calculated by AquiMod, Metran, and the national scale recharge model.

5.2 Projected recharge values

The forcing data, rainfall and potential evaporation, are altered using the change factors of the climate models (see Section **Error! Reference source not found.**). For the United Kingdom, there are two sets of monthly change factors, one used with the data driving AquiMod and Metran (Table 10), and the other used to calculate the spatially distributed recharge (Table 11). These change factors are used as multipliers to both the historical rainfall and potential evaporation values.

For the application involving AquiMod, these factors are used to alter the time series of historical rainfall and potential evaporation values used to drive the model.

When using Metran, the historical time series are altered using these factors first and then the long-term average rainfall and potential evaporation values are calculated. The recharge coefficient f_c values of the different boreholes, as calculated from the calibration of Metran model using the historical data, are then applied to calculate the projected long-term average recharge values.

The distributed recharge model ZOODRM includes the functionality of using these change factors to modify the historical gridded rainfall and potential evaporation data before using them as input to calculate the recharge. In this case, and for any simulation date, the rainfall and potential evaporation change factors for the month corresponding to the date, are used to

modify all the spatially distributed historical rainfall and potential evaporation values respectively.

Table 10 Monthly change factors as multipliers used for the borehole data

	Scenario	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Rainfall	1° Min	1.087	0.956	0.994	1.072	0.888	0.909	0.836	0.988	1.017	1.106	0.962	1.031
	1° Max	1.140	1.012	1.033	1.045	1.022	0.863	1.086	0.953	0.995	1.067	1.148	1.053
	3° Min	0.936	1.056	0.994	1.153	1.063	0.900	0.846	0.721	0.854	0.970	1.047	1.116
	3° Max	1.191	1.177	0.989	1.014	0.949	0.986	1.473	1.145	1.173	1.074	1.152	1.112
PE	1° Min	1.082	1.082	1.062	1.089	1.091	1.061	1.078	1.083	1.082	1.063	1.049	1.076
	1° Max	1.049	0.993	1.014	1.007	1.019	1.013	1.021	1.015	1.029	1.028	1.020	1.026
	3° Min	1.034	1.057	1.039	1.056	1.060	1.086	1.085	1.091	1.109	1.097	1.064	1.066
	3° Max	1.072	1.070	1.055	1.071	1.105	1.106	1.072	1.083	1.082	1.076	1.072	1.060

Table 11 Monthly change factors as multipliers used for the distributed recharge model

	Scenario	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Rainfall	1° Min	1.086	0.953	0.975	1.064	0.918	0.914	0.856	0.973	1.008	1.103	0.976	1.038
	1° Max	1.132	1.090	1.008	0.899	1.034	1.087	1.310	0.983	1.020	1.006	1.012	1.025
	3° Min	1.156	1.118	1.033	1.011	0.914	0.821	0.908	0.656	0.821	0.986	0.980	1.181
	3° Max	1.192	1.131	0.960	0.990	0.899	0.957	1.437	1.109	1.134	1.068	1.139	1.106
PE	1° Min	1.081	1.081	1.059	1.089	1.091	1.061	1.078	1.083	1.085	1.063	1.049	1.076
	1° Max	1.051	1.036	1.020	1.039	1.051	1.049	1.031	1.043	1.054	1.039	1.044	1.034
	3° Min	1.016	1.031	1.021	1.029	1.038	1.029	1.047	1.057	1.059	1.059	1.040	1.045
	3° Max	1.070	1.066	1.051	1.071	1.105	1.106	1.072	1.083	1.083	1.076	1.072	1.060

Figure 11 shows the historical and future long-term average recharge values calculated using the best performing AquiMod model. It is clear that the highest reduction in recharge values are observed when the 3° Min rainfall and evaporation data are used, while the highest increase in recharge values are observed when the 3° Max rainfall and potential evaporation data are used.

When the 1° Min scenario data are used, all the boreholes show reduction in recharge values with the highest reduction observed at Alestonefield borehole (-4%) and then at Pant Y Lladron borehole (-3.3%) and the smallest reduction is observed at Hucklow South borehole (-2%). When the 1° Max scenario data are used, all the boreholes show increase in recharge values with the smallest increase observed at Hucklow South borehole (6.3%) and then at Alestonefield borehole (6.5%) and the highest increase is observed at Pant Y Lladron borehole (7.4%).

When the 3° Min scenario data are used, all the boreholes show reduction in recharge values with the highest reduction observed at Alestonefield borehole (-7.3%) and then at PantYLladron borehole (-6.8%) and the smallest reduction is observed at Hucklow South borehole (-4%). When

the 3° Max scenario data are used, all the boreholes show increase in recharge values with the smallest increase observed at Pant Y Lladron borehole (18.3%) and Hucklow South and Alestonefield boreholes both showing an increase of 15.2%.

Projected recharge values calculated by Metran at Pant Y Lladron and Alestonefield boreholes are shown in Figure 12. The maximum reduction in recharge values as calculated by Metran at Pant Y Lladron borehole is -11.26 % while the maximum increase in recharge values at this borehole is as 13.8 %. Projected recharge values estimated at Alestonefield, however, shows unexpected increase compared to the historical recharge values using the data from all four scenarios. The maximum increase in recharge values of approximately 73% is produced using the rainfall and potential evaporation change factors of the 3° Max scenario.

Table 12 shows the monthly historical and future recharge values calculated at the different boreholes calculated by AquiMod. It is clear that in almost all the cases, the recharge values become lower than the historical values when the 1° Min and 3° Min data are used and they become higher than the historical values when the 1° Max and 3° Max are used. The exceptions of this observation are due to the complex effect of the use of the change factors, which may reduce both the rainfall and potential evaporation at the same period but at different rates. The reduction in potential evaporation volume in one month may yield increased recharge volume even if the rainfall volume is reduced for that month.

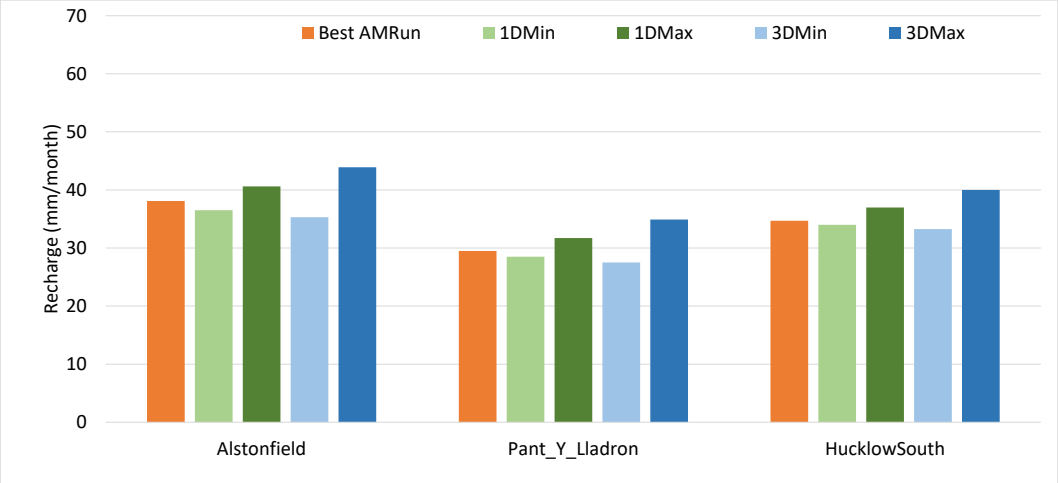


Figure 11 Historical (orange) and future recharge values (blue and green) as produced by the best performing AquiMod model.

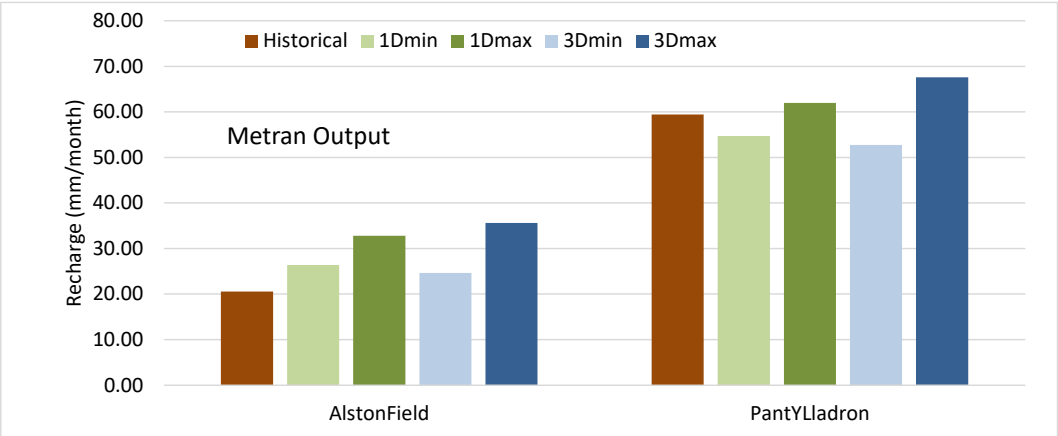
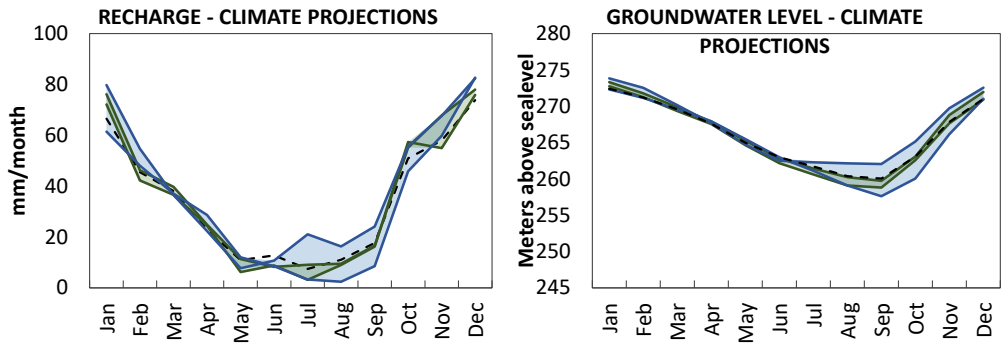


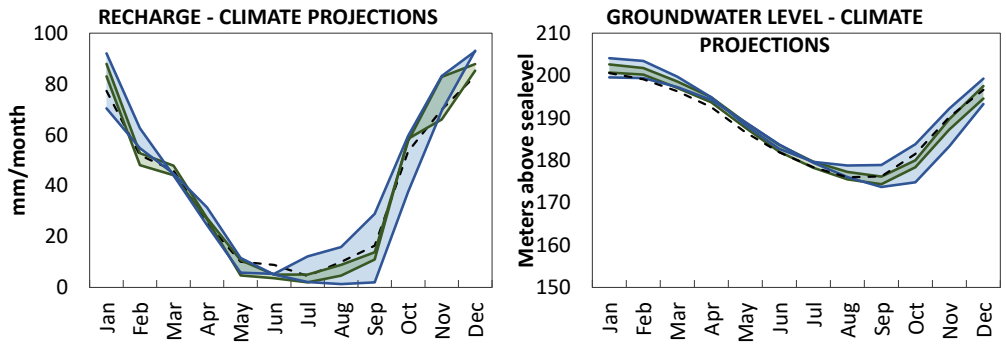
Figure 12 Historical (orange) and future recharge values (blue and green) produced by Metran.

Table 12 Monthly recharge values estimated using the historical and the projected forcing data. Dotted line is the monthly historical recharge values. Green shaded area shows the 1° Min and Max monthly recharge values and the blue shaded area shows the 3° Min and Max monthly recharge values

Hucklow South



Alstonefield



Pant Y Lladron

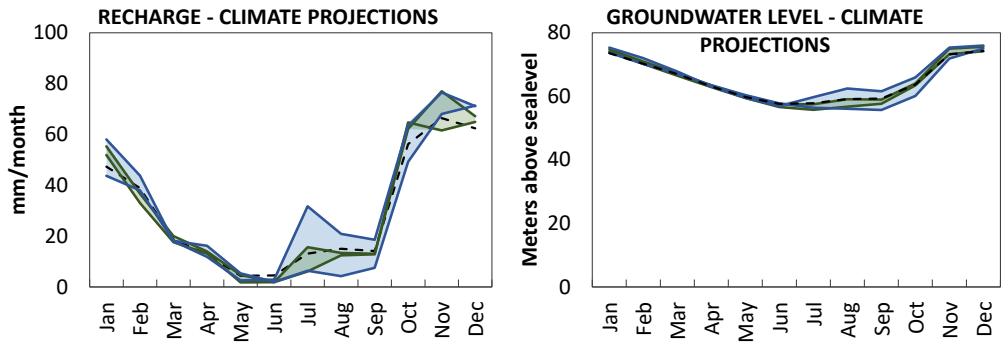


Table 13 shows maps of the spatially distributed recharge values calculated over the Devonian sandstone / Carboniferous Limestone aquifer. The plots are for the historical potential recharge values as well as those calculated using the distributed recharge model but with rainfall potential evaporation data altered using the 1° Min, 1° Max, 3° Min, and 3° Max UK change factors. The differences in the maps are not clear, however, the 1° Min and 3° Min data produce drier recharge maps and the 1° Max and 3° Max data produce wetter recharge maps as confirmed with the difference maps listed in Table 14.

Table 15 shows the average, maximum, and the standard deviation values calculated using the pixel values of the maps shown in Table 13. Looking at the average values, it is clear that there is reduction in recharge when the 1° Min or the 3° Min data are used compared to the historical recharge. The maximum of the pixel values of the 1° Min map is higher than the maximum of the pixel values of the 3° Min map as expected. The average recharge values of the pixel values of the 1° Max and 3° Max maps are both higher than the average from the historical map as expected. The maximum value from these two maps are also higher than the maximum obtained from the historical. Finally, there is little difference in the standard deviation values shown in Table 15 indicating that the spatial distribution of recharge values is not notably different between the different scenarios.

Table 13 Spatially distributed historical and projected recharge values

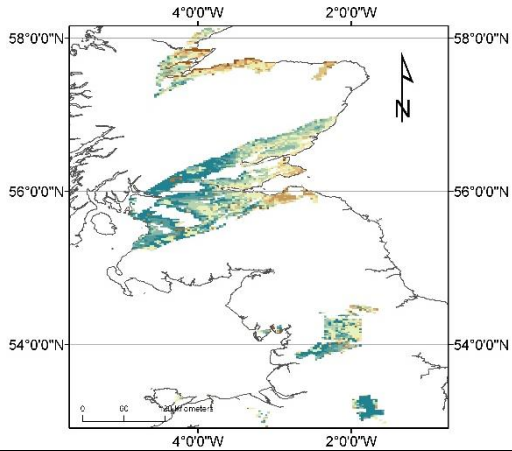
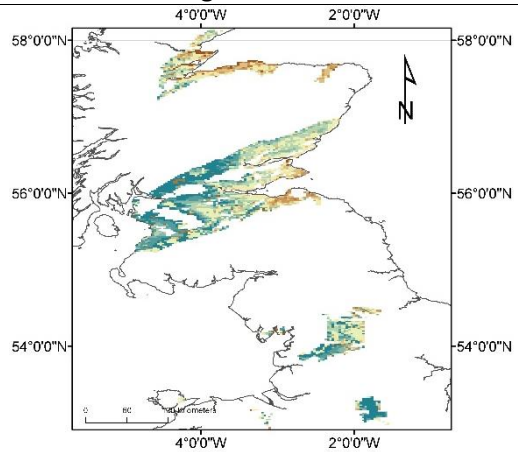
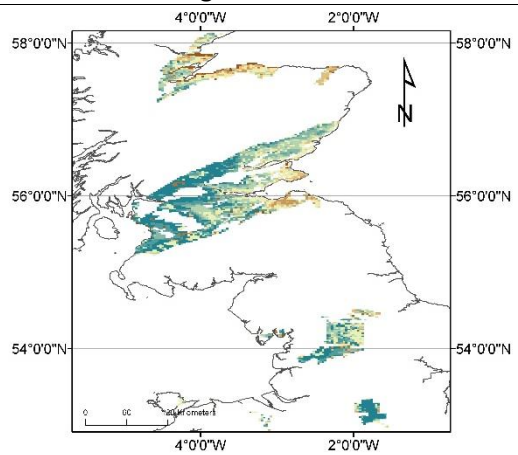
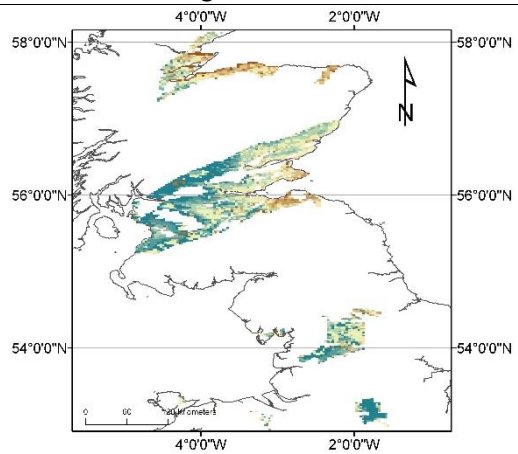
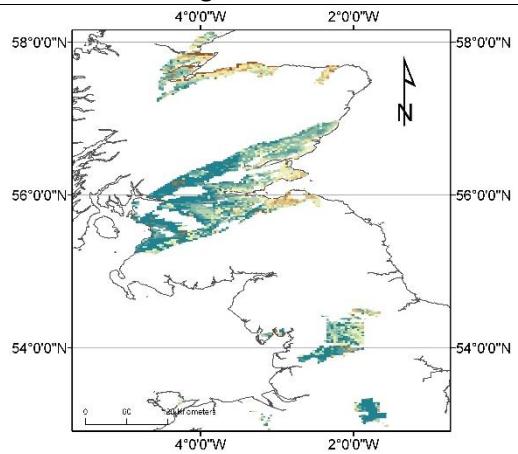
Historical	Legend: Recharge (mm/day)
	**Recharge (mm/day)** 0 - 0.18 0.181 - 0.337 0.338 - 0.471 0.472 - 0.612 0.613 - 0.761 0.762 - 0.91 0.911 - 1.07 1.08 - 1.24 1.25 - 1.45 1.46 - 2
CC scenario: 1 degree min	CC scenario: 1 degree max
	
CC scenario: 3 degrees min	CC scenario: 3 degrees max
	

Table 14 Differences between the projected and historical recharge values calculated as projected values minus historical values

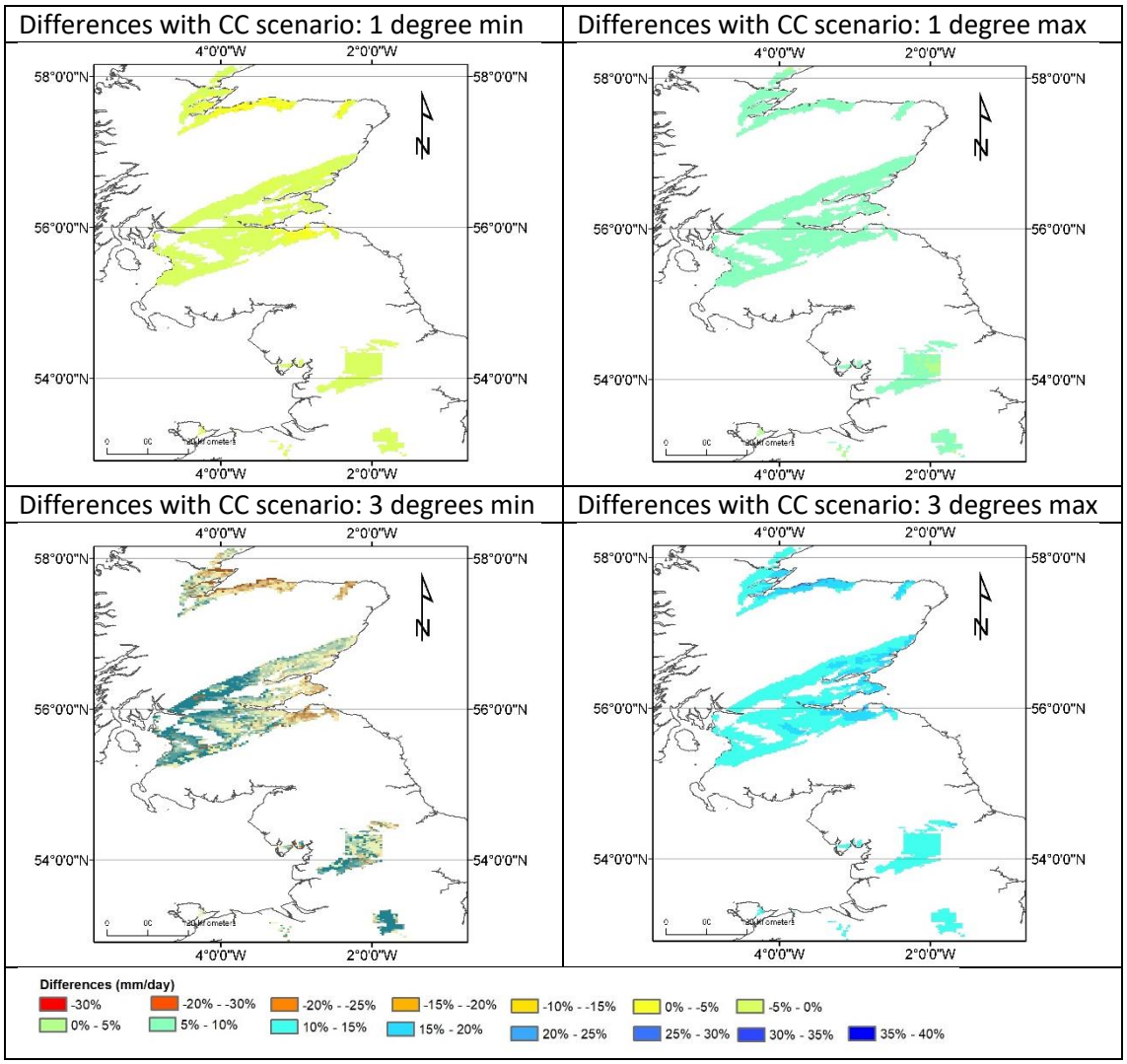


Table 15 Statistical information about the maps shown in Table 13

Map	Average recharge (mm/day)	Maximum recharge (mm/day)	Standard deviation (mm/day)
Historical	1.12	4.73	0.57
CC scenario: 1 degree min	1.087	4.71	0.567
CC scenario: 1 degree max	1.178	4.964	0.601
CC scenario: 3 degrees min	1.081	4.667	0.561
CC scenario: 3 degrees max	1.260	5.227	0.6334

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APPENDICES

Appendix A: AquiMod methodology

AquiMod is a lumped parameter computer model that has been developed to simulate groundwater level time series at observational boreholes (Mackay et al., 2014a). It is based on hydrological algorithms that simulates the movement of groundwater within the soil zone, the unsaturated zone, and the saturated zone. The lumped models neglect complexities included in distributed groundwater models but maintains some of the fundamental physical principles that can be related to the conceptual understanding of the groundwater system (Mackay et al., 2014b).

While AquiMod was originally designed to capture the behaviour of a groundwater system through the analysis of groundwater level time series, it can produce the infiltration recharge values and groundwater discharges from the aquifer as a by-product. AquiMod is driven by complete time series of forcing data for either historical or predicted future conditions. Running AquiMod in predictive mode can be used to fill in gaps in historical groundwater level time series, or calculate future groundwater levels. In addition to groundwater levels, it also provides predictions of historical and future recharge values and groundwater discharges. In the current application we use calibrated AquiMod models to estimate the recharge values at selected boreholes.

AquiMod consists of three modules (Figure A1). The first is a soil water balance module that calculates the amount of water that infiltrates the soil as well as the soil storage. The second module controls the movement of water in the unsaturated zone, mainly it delays the arrival of infiltrating water to the saturated zone. The third module calculates the variations in groundwater levels and discharges. The model executes the modules separately following the order listed above.

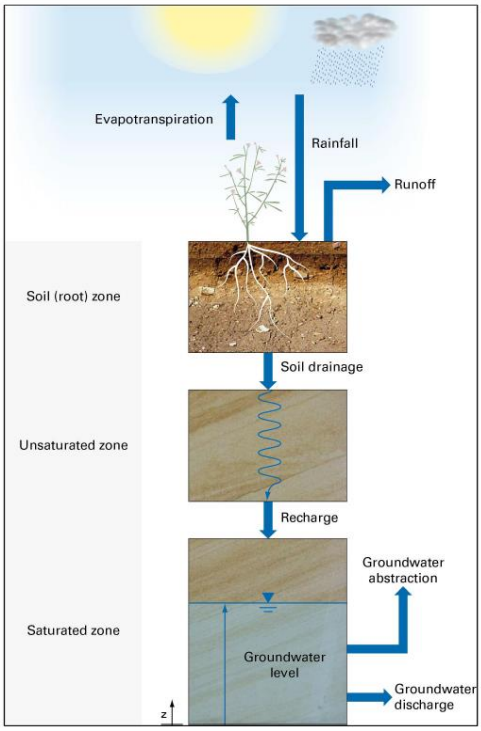

Figure A1 Generalised structure of AquiMod (after Mackay et al., 2014a)

The soil moisture module

There are several methods available in AquiMod that can be used to calculate the rainfall infiltration into the soil zone. In this study we use the FAO Drainage and Irrigation Paper 56 (FAO, 1988) approach. In this method, the capacity of the soil zone, from which plants draw water to evapo-transpire, is calculated first using the plants and soil characteristics. Evapo-transpiration is calculated according to the soil moisture deficit level compared to two parameters: Readily Available Water (RAW) and Total Available Water (TAW). These are a function of the root depth and the depletion factor of the plant in addition to the soil moisture content at field capacity and wilting point as shown in Equations A1 and A2.

$$TAW = Z_r(\theta_{fc} - \theta_{wp}) \qquad \text{Equation A1}$$

$$RAW = p \cdot TAW \qquad \text{Equation A2}$$

Where Z_r [L] and p [-] are the root depth and depletion factor of a plant respectively, θ_{fc} [L^3 L^{-3}] and θ_{wp} [L^3 L^{-3}] are the moisture content at field capacity and wilting point respectively.

The FAO method is simplified by Griffiths et al. (2006) who developed a modified EA-FAO method. In this method the evapotranspiration rates are calculated as a function of the potential evaporation and an intermediate soil moisture deficit as:

$$\begin{aligned} e_s &= e_p \left[\frac{s_s^*}{TAW - RAW}\right]^{0.2} && s_s^* > RAW \\ e_s &= e_p && s_s^* \leq RAW \\ e_s &= 0 && s_s^* \geq TAW \end{aligned} \qquad \text{Equation A3}$$

Where e_s [L] is the evpo-transpiration rate, e_p [L] is the potential evaporation rate and s_s^* [L] is the intermediate soil moisture deficit given by

$$s_s^* = s_s^{t-1} - r + e_p \qquad \text{Equation A4}$$

Where r [L] is the rainfall at the current time step and s_s^{t-1} [L] is the soil moisture deficit calculated at the previous time step.

The new soil moisture deficit is then calculated from:

$$s_s = s_s^{t-1} - r + e_s \qquad \text{Equation A5}$$

Griffiths et al. (2006) proposed that the recharge and overland flow are only generated when the calculated soil moisture deficit becomes zero. The remaining volume of water, the excess water, is then split into recharge and overland flow using a runoff coefficient. In AquiMod a baseflow coefficient is used to reflect the fact that a groundwater discharge is calculated rather than overland water. In this application, the baseflow coefficient is one minus the runoff coefficient.

The unsaturated zone module

The AquiMod version used in this study to simulate the movement of groundwater flow within the unsaturated zone is based on a statistical approach rather than a process-based approach. This method distributes the amount of rainfall recharge over several time steps where the soil drainage for each time step is calculated using a two-parameter Weibull probability density function. The Weibull function can represent exponentially increasing, exponentially decreasing, and positively and negatively skewed distributions. This can be used to focus the soil drainage over earlier or later time steps or to spread it over a number of time steps after the infiltration occurs. The shape of the Weibull function is controlled by two parameters, k and λ as shown in Equation A6.

$$f(t,k,\lambda) = \begin{cases} \frac{k}{\lambda}\left(\frac{t}{\lambda}\right)^{k-1} e^{-(t/\lambda)^{k-1}} & t>0 \\ 0 & t\leq 0 \end{cases} \qquad \text{Equation A6}$$

Where k and λ are two parameters the values of which are calculated during the calibration of the model and t is the time step.

The saturated zone module

AquiMod considers the saturated zone as a rectangular block of porous medium with dimensions L and B as its length and width [L] respectively. This block is divided into a number of layers, each has a defined hydraulic conductivity value, a storage coefficient value, and a discharging feature. The number of layers define the structure of the saturated module used in the study.

The mass balance equation that gives the variation of hydraulic head with time is given by:

$$SLB\frac{dh}{dt} = RLB - Q - A \qquad \text{Equation A7}$$

Where:

S is the storage coefficient of the porous medium [-]

h is the groundwater head [L]

t is the time [T]

R is the infiltration recharge [L T^{-1}]

Q is the discharge out of the aquifer [L T^{-1}]
A is the abstraction rate [L T^{-1}]

It must be noted that in a multi-layered groundwater system as shown in Figure A2, we calculate one groundwater head (h) for the whole system. The discharges (Q) from Outlet 1, 2, etc. are calculated using the Darcy law. The total discharges can be summarised using the following equation:

$$Q = \sum_{i=1}^{m} \frac{T_i B}{0.5\ L} \Delta h_i \qquad \text{Equation A8}$$

Where:
m is the number of layers in the groundwater system [-]
T_i is the transmissivity of the layer i [L T^{-2}]
Δh_i is the difference between the groundwater head h and z_i, the elevation of the base of layer i

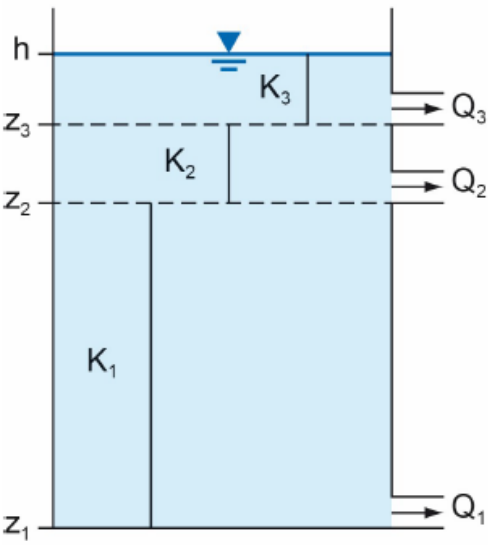

Figure A2 Representation of the saturated zone using a multi-layered groundwater system

Substituting Equation A8 into Equation A7 yields a numerical equation in the form:

$$S \frac{(h-h^*)}{\Delta t} = R - \sum_{i=1}^{m} \frac{T_i}{0.5\ L^2} \Delta h_i - \frac{A}{LB} \qquad \text{Equation A9}$$

Equation A9 is an explicit numerical equation that allows the calculation of the groundwater head h [L] at any time and using time steps of Δt [T]. In this equation h^* [L] is the groundwater head calculated at the previous time step and the term Δh_i [L] is calculated as $(h^* - z_i)$.

The terms S, T_i, and L are optimised during the calibration of the model. A groundwater system can be specified with one storage coefficient as shown in the equations above or with different storage coefficient values for the different layers. Several saturated modules are included in AquiMod to provide this flexibility and the model user can select the model structure that represent the conceptual understanding best.

Limitations of the model

AquiMod is a lumped groundwater model that aims at reproducing the behaviour of the observed groundwater levels. It tries to encapsulate the conceptual understanding of a groundwater system in a simple numerical representation. The model results have to be therefore discussed, taking this into consideration. For example, the model represents the groundwater system as a closed homogeneous medium, with no impact from any outer boundary or feature, whether physical or hydrological, such as the presence of rising and falling river stage.

Vertical heterogeneity can be accounted for by using multi-layered groundwater module structure. However, this model setting does not provide any information about the vertical connections between the layers as the discharge from all the layers is calculated using one representative groundwater head value. In other words, it is assumed that all layers are in perfect hydraulic connection.

As mentioned before, the model is designed to simulate the groundwater levels. However, it produces the recharge values and groundwater discharges as by products. In this application we use the calibrated model to calculate recharge. The mass balance equation (Equation A7) shows that recharge is a function of transmissivity and storage coefficient values, which are estimated during the calibration process of the model, i.e. they are not parameters with fixed values provided by the user. The inter-connections between these parameters leads to uncertainties in the estimated recharge values as a high storage coefficient value can produce a high recharge estimate and vice versa. To overcome this problem, it is suggested that the recharge values estimated by AquiMod are always presented as a range of possibilities rather than an absolute value. This can be achieved by estimating the recharge values from all the models that have a performance measure above than a threshold that is deemed acceptable by the user. The recharge estimates can then be presented as an average of all estimates and values corresponding to selected percentiles.

Model input and output

AquiMod includes a number of methods that calculates rainfall recharge as well as a number of model structure from which the user can select what better suits the case study.

Model input consists time series of forcing data including rainfall and potential evaporation, time series of anthropogenic impact mainly groundwater abstraction and time series of groundwater levels that will be used to calibrate the model. These time series must be complete, i.e. a value is available at every time step except the groundwater level time series, which can include missing data. The time step can be one day or multiple of days, and the model automatically calculate the size of the time step based on the input data time series.

The model is run first in calibration mode where a range of parameter values are specified for the different parameters included in the three model modules. A Monte Carlo approach is used to select the best parameter values. The performance of the model is measured by comparing the simulated groundwater levels to the observed ones using the Nash Sutcliff Efficient (NSE) or

the Root Mean Squared Error (RMSE) performance measures. The parameter set that produces the best model performance is selected to run the model in evaluation mode.

When the model is run in evaluation mode, it produces output files that give recharge values, groundwater levels and groundwater discharges time series with time as specified in the input file. The number of output files is equal to the number of acceptable models set by the user.

Appendix B: Metran methodology

Metran applies transfer function noise modelling of (groundwater head) time series with usually daily precipitation and evaporation as input (Zaadnoordijk et al., 2019). The setup is shown in the Figure B1. If time series of other influences on the groundwater head are available, these contributions can be added to the deterministic part of the model. The stochastic part is the difference between the total deterministic part and the observations (the residuals). The corresponding input of the noise model should have the character of white noise.

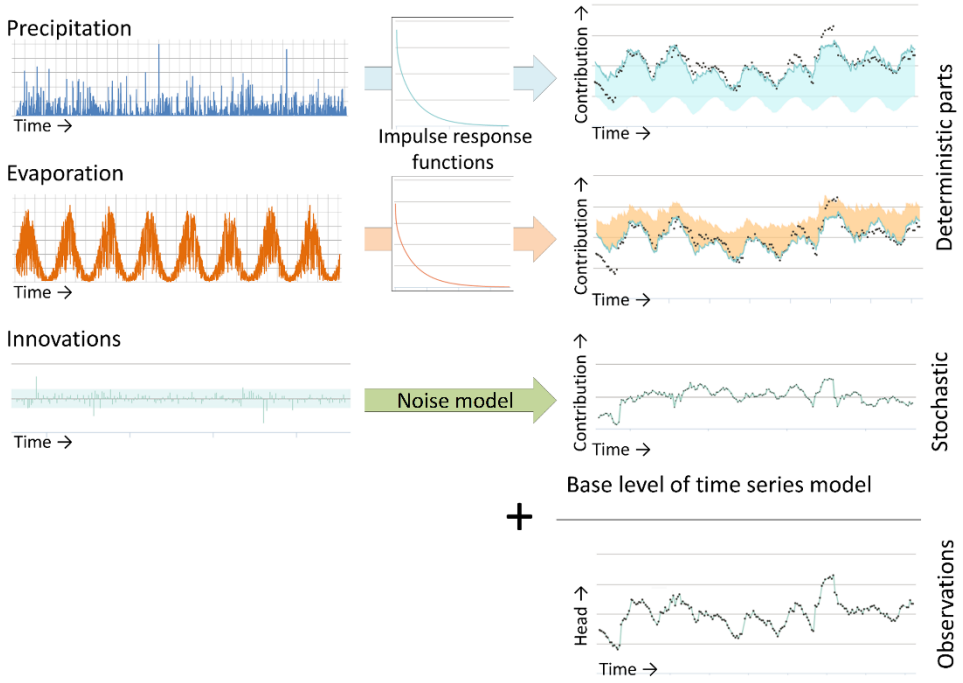

Figure B1 Illustration of METRAN setup

The stochastic part is needed because of the time correlation of the residuals, which does not allow a regular regression to obtain the parameter values of the transfer functions.

The incomplete gamma function is used as transfer function. This is a uni-modal function with only three parameters that has a quite flexible shape and has some physical background (Besbes & de Marsily, 1984). The evaporation response is set equal to the precipitation response except for a factor (fc). The noise model has one parameter that determines an exponential decay. Thus, for the standard setup with precipitation and evaporation, there are five parameters that have to be determined from the comparison with the observations. Three parameters regarding the precipitation response, the evaporation factor, and the noise model parameter (actually, the time series model has a fifth parameter, the base level, but this is determined from the assumption that the average of the calculated heads is equal to the average of the observations). There are three extra parameters for each additional input series, such as pumping.

Limitations

Metran's time series model is linear. So, the model creation breaks down when the system is strongly nonlinear. This can occur e.g. when drainage occurs for high groundwater levels, when the ratio between the actual evapotranspiration and the inputted reference evaporation varies strongly, or when the groundwater system changed during the simulated period.
Metran is not able to find a decent time series model when the response function is not appropriate for the groundwater system. An example of this is a system with a separate fast and slow response as was found for a French piezometer in the Avre region, as is illustrated in Figure B2.

Finally, the parameter optimization of Metran uses a gradient search method in the parameter space, so it can be sensitive to initial parameter values in finding an optimal solution.

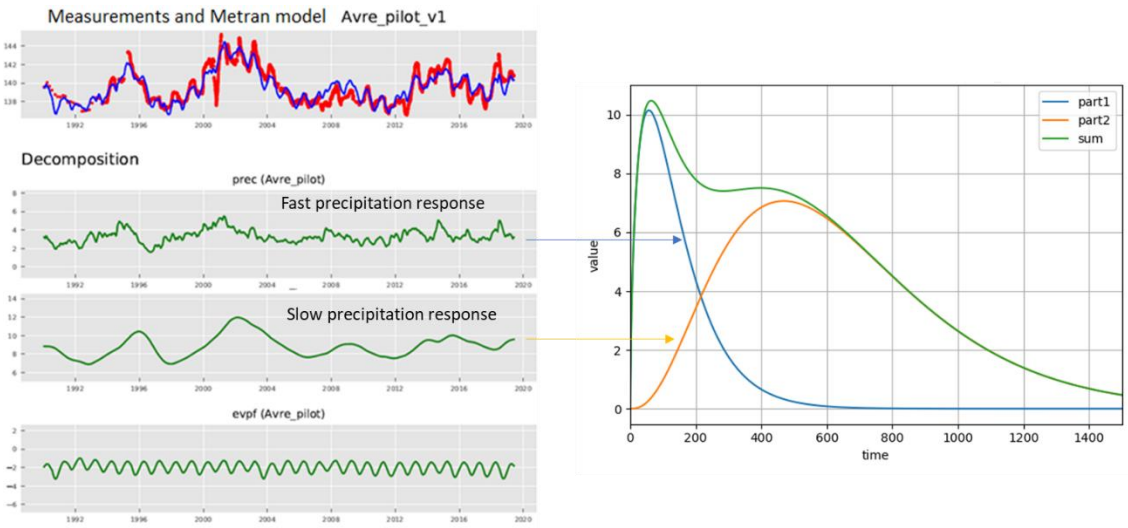

Figure B2. An example where the response function implemented in METRAN is not suitable for the groundwater system

Time step

Metran has been designed to work with explanatory series that have a daily time step. However, it has been adapted so that other time step lengths can be applied; although Metran still has the limitation that the explanatory variables have a constant frequency. For the TACTIC simulations of series with monthly or decadal meteorological input series, the time step has been set to 30 and 10 days, respectively. This time step has been applied from the end date backward.
Note that the heads may be irregular in time as long as the frequency is not greater than the frequency of the explanatory series.

Model output

The evaporation factor fc gives the importance of evapotranspiration compared to precipitation. The parameter M_0 gives the total precipitation response, which is equal to the area below the impulse response function and the final value of the step response function.

The average response time is another characteristic of the precipitation response. The influence is illustrated in Figure B3 with the impulse response functions and head time series for two models with very different response times for time series of SGU in Sweden.

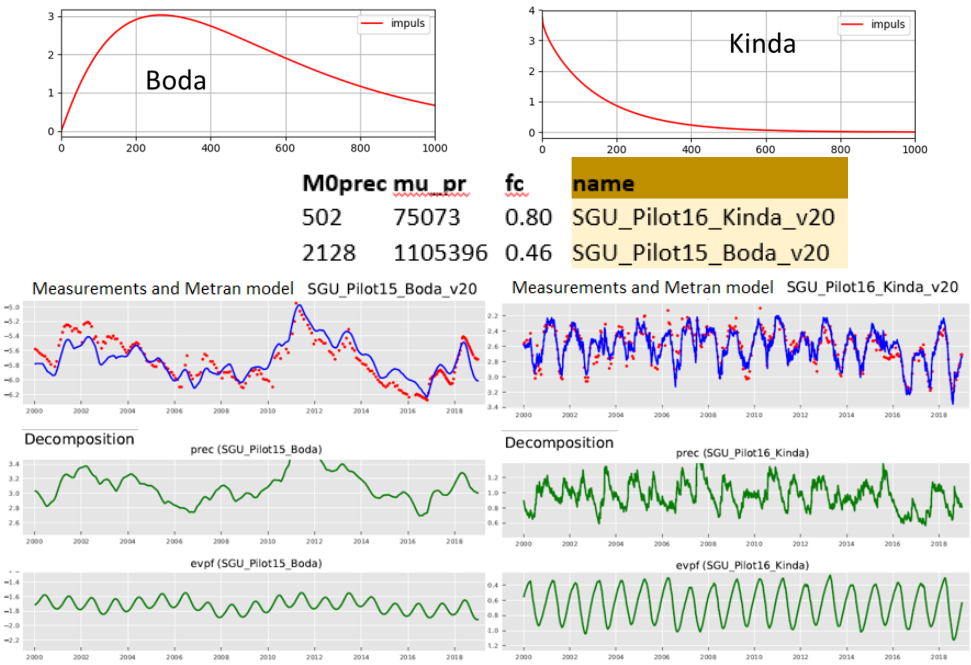

Figure B3 Illustration of Metran output for two case studies in Sweden with different response times.

Model quality

Metran judges a resulting time series model according to a number of criteria and summarizes the quality using two binary parameters Regimeok, Modok (see Zaadnoordijk et al., 2019):

- Regimeok =1 : highest quality
- Modok = 1 (and Regimeok = 0) : ok
- Both zero = model quality insufficient

More detailed information on the model quality is given in the form of scores for two information criteria (AIC and BIC), a log likelihood, R2, RMSE, and the standard deviations and correlations of the parameters.

Recharge

Although the transfer-noise modelling of Metran determines statistical relations between groundwater heads and explanatory variables, we like to think of the results in physical terms. It is tempting to interpret the evaporation factor, as the factor translating the reference into the actual evapotranspiration. Then, we can calculate a recharge as

$$R = P - fE \qquad \text{Equation B1}$$

where R is recharge, P precipitation, E evapotranspiration, and f the evaporation factor.

Following the definitions used in the TACTIC project, this recharge R actually is the effective precipitation. It is equal to the potential recharge when the surface runoff is negligible. This in turn is equal to the actual recharge at the groundwater table if there also is no storage change or interflow. In such cases it may be expected that this formula indeed corresponds to the meteorological forcing of the groundwater head in a piezometer, so that it gives a reasonable estimate of the recharge. Obergfell et al. (2019) showed this for an area on an ice pushed ridge in the Netherlands. However, this assumes that all precipitation recharges the groundwater, which cannot be done in many places.

In Dutch polders with shallow water tables and intense drainage networks, it is reasonable to assume that the actual evapotranspiration is equal to the reference value. In that case, the factor f becomes larger than 1 because 1 mm of evaporation has less effect than 1 mm of precipitation (because part of the evaporation does not enter the ground but is immediately drained to the surface water system). In that case, we can calculate recharge as:

$$R = P - fE \qquad f \leq 1$$
$$R = P/f - E \qquad f > 1 \qquad \text{Equation B2}$$

These simple formulas can be applied easily for the situations currently modelled in Metran and for the simulations that are driven by future climate data using the delta-change climate factors. However, it is noted that it is a crude estimate using assumptions that are easily violated. Because of this, the equations should be applied only to long term averages using only models of the highest quality.