British Geological Survey

AquiMod 2 User Manual

Environmental Change, Adaptation and Resilience Programme
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BRITISH GEOLOGICAL SURVEY

ENVIRONMENTAL CHANGE, ADAPTATION AND RESILIENCE PROGRAMME

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AquiMod 2 User Manual

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AquiMod logo

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Summary

This user manual describes the second version of AquiMod (AquiMod 2), a simple lumped groundwater level simulation model. It covers all of the existing features of AquiMod and the new features in AquiMod 2. Experienced users will be familiar with much of the content of this user manual and will not need to read it in its entirety. Instead, they may wish to refer to the 'Release Notes' and 'Checklist for moving from AquiMod to AquiMod 2' sections which can be found at the front of this document, and which include links to the sections of the manual that are relevant to the new features. They may also wish to work through the two additional tutorials in this user manual which cover some of the new features in AquiMod 2 (sections 6.4 and 6.5).

As well as the addition of tutorial material and descriptive text for new features, the text covering existing features has also been revised in some cases for the benefit of the reader. This includes, for example, revised mathematical notation to provide consistency across the different module components.

All examples shown were undertaken on a computer running Windows 10 (64-bit). Consequently, some aspects of running AquiMod 2 may differ when using a different version of the Windows operating system.

AquiMod 2 Release Notes

- Setup wizard for easier installation/uninstallation across windows versions (section 2.1).
- New NSSS and SMAP soil zone components (sections 0 and 0).
- Automated selection of n parameter for Weibull unsaturated zone component for faster runtime (section 0).
- New Q3K3S3, Q2K2S2, Q1K2S2 and SA1D saturated zone components (sections 0, 0 and 3.3.8).
- New F-score and weighted NSE-F-score objective functions (section 4.1).
- New Shuffled Complex Evolution mode for global parameter optimisation (section 0).
- New soil water content column in Observations.txt file with ability to impose soil moisture conditions (section 5.2.1).
- Calibration and evaluation input file templates are generated by AquiMod 2 when not provided by the user (section 5.3).
- Ability to calibrate/evaluate against soil moisture data (see tutorial in section 6.4 for worked example).
- Input file templates and output files have been updated so that variable notation is consistent with model equations in this report (Appendix 1).
- All soil zone components now output volumetric soil water content rather than soil moisture deficit (Appendix 1).
- Improved handling and reporting of user input errors.

Checklist for moving from AquiMod to AquiMod 2

When using the AquiMod 2 software with models originally configured for AquiMod 1.0, make sure to consider the following:

- When using the Weibull unsaturated zone component, the n parameter no longer needs to be specified in the calibration and evaluation input files (section 0).
- Observations.txt should include an additional column for volumetric soil water content observations (section 5.2.1)
- Input.txt file structure and contents should be updated according to section 5.2.2.

1 Overview

AquiMod is a lumped parameter computer model that has been developed to simulate groundwater level time series at observation boreholes in aquifers by linking simple hydrological algorithms that simulate soil drainage, the transfer of water through the unsaturated zone, and groundwater flow. It runs on a Windows PC through the command prompt and is configured using a series of text files. The simple structure of AquiMod makes it easy to use in comparison to more complex distributed models, and therefore should be accessible to those users who are new to the field of groundwater and hydrological modelling. It includes a number of alternative conceptual modelling approaches of varying complexity, but which are all based on hydrological process understanding. It is also extremely efficient and quick to run. These features make it ideal for delivering groundwater level simulations quickly and the code also lends itself for more computationally demanding multi-simulation tasks such as global parameter sensitivity and uncertainty analysis. Since the release of AquiMod 1.0 in 2014, the code has been applied widely in the United Kingdom for operational seasonal and flood forecasting of groundwater levels (Mackay et al., 2015), groundwater level record reconstruction (Jackson et al., 2016) and climate change impact assessment (Hannaford et al., 2022a). It has also been used in other geographical settings including Sub-Saharan Africa (Ascott et al., 2020) and the Philippines (Mackay et al., 2022) and continues to be used to teach concepts of subsurface flow and modelling to a range of audiences including Earth Science undergraduates and within the water sector.

During these applications, we've made a number of modifications to the source code including adding new model structures, improving the model runtime and providing new functionality for model calibration and evaluation. Some of these modifications were purely experimental and not all of them have stood the test of time. AquiMod 2 only includes those updates which we have judged to provide a genuine benefit to users and which we have been tested sufficiently to ensure overall code robustness. We use the term 'AquiMod' when referring to both versions of the code generally and 'AquiMod 2' when specifically referring to this new version. The main features of AquiMod 2 include:

- Fast simulation of groundwater level time series
- Flexible time stepping
- Monte Carlo parameter sampling
- Automated global parameter optimisation
- Modular structure with multiple process representations
- Choice of objective functions to evaluate model efficiency

1.1 INTENDED USE

AquiMod can be applied to any groundwater catchment around an observation borehole with observed groundwater level time series data. It can be calibrated against these data and used to provide information on the behaviour of groundwater levels beyond observational records. The model has been used in this way for a number of applications, including reconstructing groundwater level records, long term projections of groundwater levels under climate change, and forecasting groundwater levels into the near future using meteorological forecasts. Of course, this list of applications is not absolute and users are encouraged to experiment with the software. However, it is important to consider the limitations of the AquiMod when deciding if it is suitable for your intended use. Please refer to a summary of these limitations in (Table 1).

Table 1: Considerations and potential limitations when applying AquiMod for groundwater level simulation.

Consideration	Limitation
Lumped model structure	AquiMod lumps the catchment area into a single response unit which is characterised by a groundwater level borehole hydrograph. It treats each input variable, catchment parameter and output variable as spatially uniform and, therefore, cannot provide information on spatial heterogeneity within a given catchment area.
Time series data	AquiMod needs either observed groundwater level or soil moisture time series to evaluate the model. It also needs rainfall and potential evapotranspiration (PET) time series to drive the model.
Model boundary	AquiMod was designed to be used near boreholes with a well-defined groundwater catchment that is assumed to be static with negligible flow across the lateral boundaries.
Influence of nearby abstractions	AquiMod has not been designed to accurately account for the influence of significant groundwater abstractions in the vicinity of a borehole and, therefore, applications of AquiMod in these regions are generally not recommended.

1.2 GENERALISED STRUCTURE

AquiMod consists of three modules (Figure 1). The first is a soil water balance module that partitions rainfall between evapotranspiration, runoff, and soil drainage. This module simulates the water balance within the soil root zone where drainage is defined as the water that percolates downwards beyond the base of the root zone and is no longer available for evapotranspiration. Drainage from the soil is then attenuated through an unsaturated zone module which represents percolation to the groundwater table as recharge. This recharge is input to the saturated zone module that simulates aquifer storage and subsequent discharge. It is the saturated zone module that simulates groundwater level fluctuations over time.

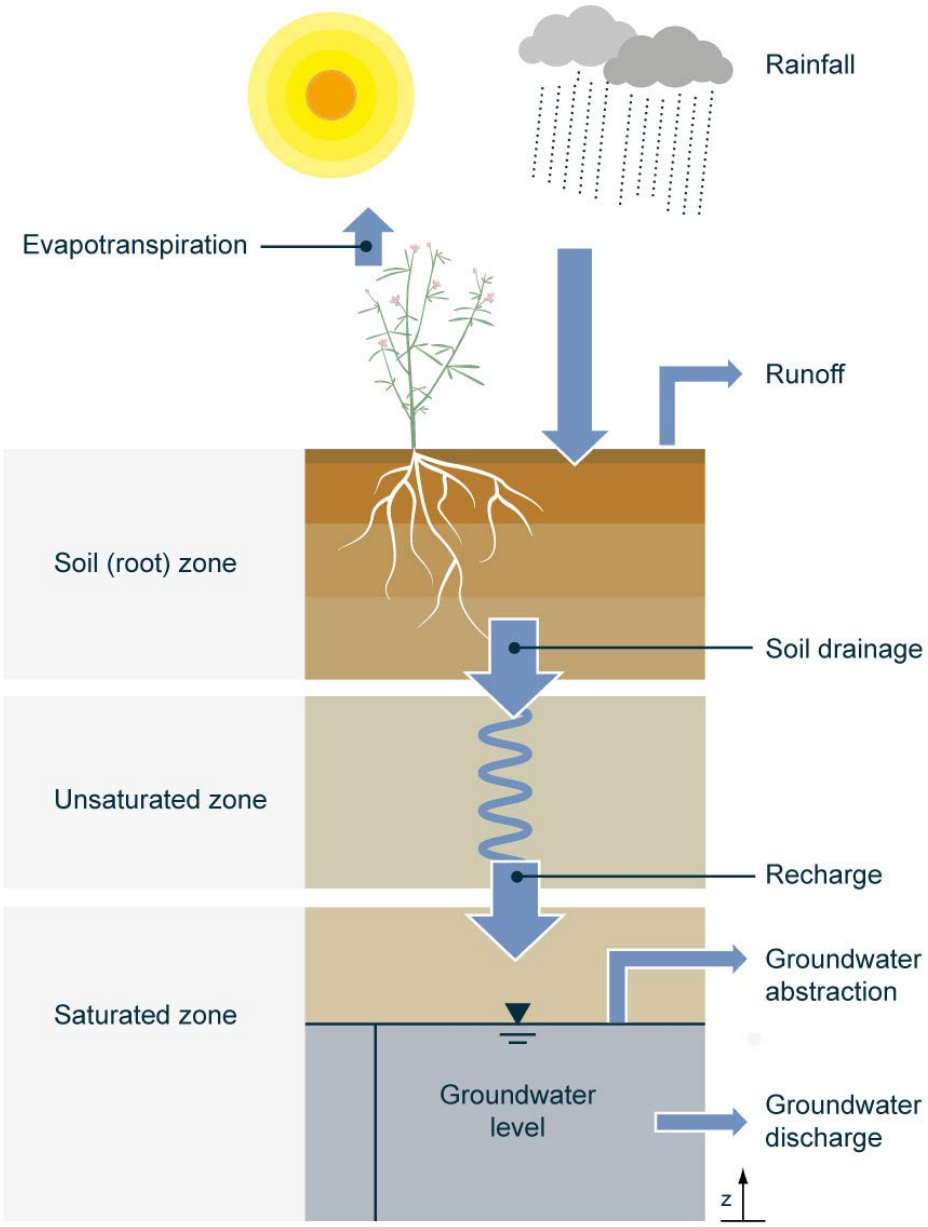

Figure 1: Generalised structure of AquiMod.

2 Getting started

2.1 INSTALLATION

Before starting, you'll need to download the AquiMod 2 setup file which is available directly from the British Geological Survey website here. To install the software, run this setup file. This will open a setup wizard.

- First you will need to specify an **installation directory**.
- You will then be asked if you would like to run the 'Add to path' task (Figure 2). **Ensure that this option is checked** as this will update your system Path environment variable so that you can run AquiMod 2 from the command line. If you choose to uncheck this option, you will need to update this variable manually.
- Continue through the wizard until you reach the 'Completing the AquiMod 2 Setup Wizard' window.
- **Click Finish**.

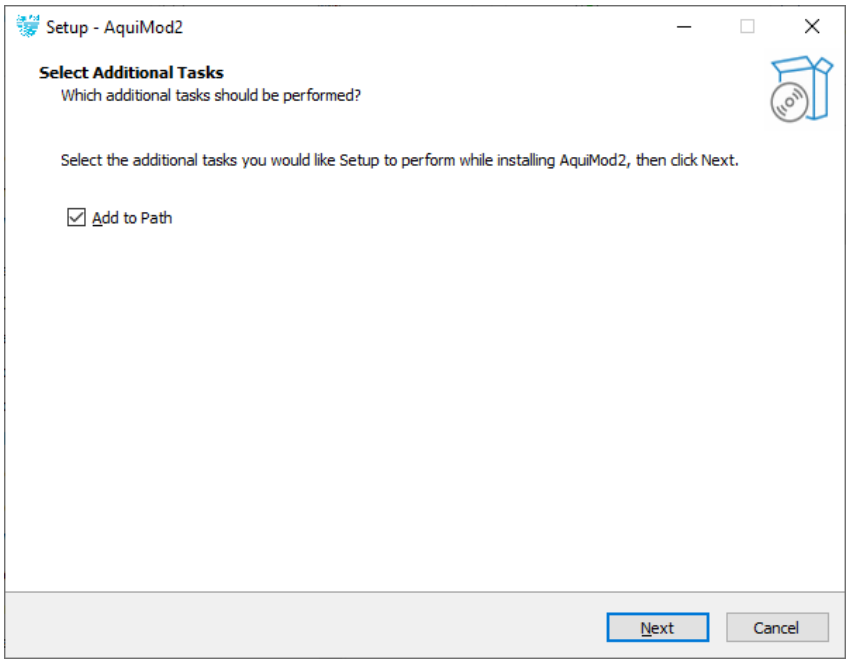

Figure 2: AquiMod 2 setup wizard 'Additional tasks' window.

AquiMod 2 is now ready to use.

The installation directory should now contain the AquiMod 2 executable along with two folders named CHexample and CFexample. These folders contain the input files for two example models which are required for the Tutorials in section 0. You may wish to copy these into a different working folder on your hard disk.

2.2 RUNNING AQUIMOD

The AquiMod2 executable (AquiMod2.exe) is run using the Windows command prompt which can be accessed by typing 'cmd' into the search bar of the Start menu and hitting the return key. Once the command prompt has loaded, AquiMod2 is run by typing 'aquimod2' and the directory address of the model files separated by a space. In the command prompt type aquimod2 followed by the location of the CHexample folder as shown in Figure 3. Note that here, the CHexample folder has been copied to the root of the C drive.

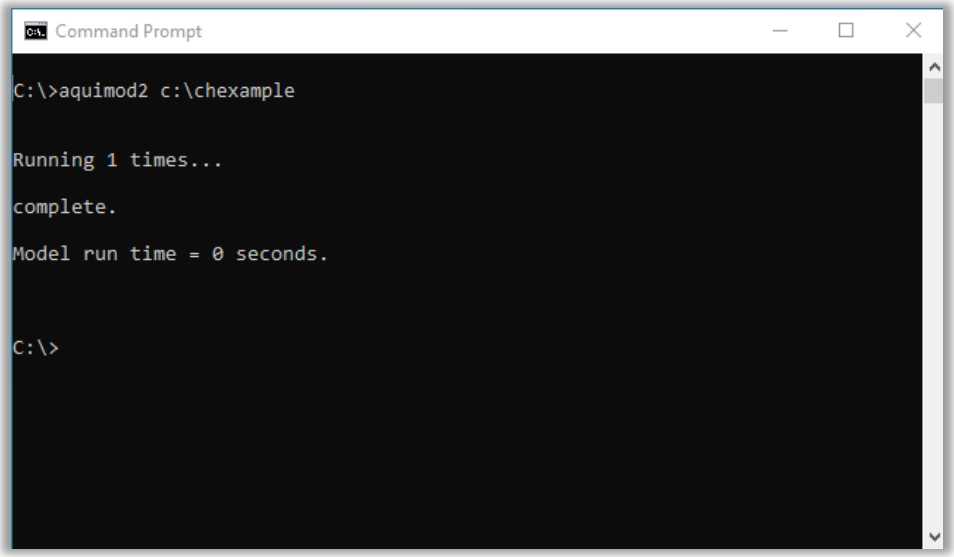

Figure 3: Running AquiMod 2 through the command prompt.

Notice that AquiMod 2 provides output messages to indicate that the model run has completed. If you navigate to the Output folder, you should see several files with the '.out' filename extension. These are output files produced by AquiMod. They are text files that can be viewed in your text editor.

3 Modules

AquiMod has three modules that represent the soil, unsaturated and saturated zone hydrology. Each module has been designed so that it can incorporate a number of possible structures (components), each based on a different conceptual representation of the process being considered, but all of which adhere to the same generalised structure outlined in section 0. Each component uses one or more parameters which can be modified to change the behaviour of the model. These parameters and the mathematical algorithms that AquiMod 2 employs are described below.

3.1 SOIL ZONE MODULE

There are three soil zone components available in the AquiMod 2 software (Table 2). All components simulate a 'lumped' soil water level, Θ [L], which represents the integrated volumetric water content of the soil, θ [-] over the soil column which extends down to the maximum root zone depth, Z_r

$$\Theta = \int_0^{Z_r} \theta \, dz \tag{1}$$

where z [L] is the depth below the ground surface. The soil is conceptualised to have a finite storage of water available to plants for uptake[1], Θ_{pu} [L] which can be quantified directly from properties of the soil. If we assume the soil is homogeneous, this can be calculated as

$$\Theta_{pu} = Z_r(\theta_{fc} - \theta_{wp}) \tag{2}$$

where θ_{fc} and θ_{wp} [-] are the soil field capacity and wilting point, respectively. This definition assumes that water storage beyond field capacity, which drains freely under gravity, is not readily available for plant uptake. If the soil water level is below field capacity, the soil is said to be in a state of moisture deficit

$$\Theta_{smd} = \Theta_{wp} + \Theta_{pu} - \Theta \tag{3}$$

where Θ_{smd} is the soil moisture deficit [L].

Soil water storage fluctuations within the root zone are calculated according to the mass conservation statement

$$\frac{d\Theta}{dt} = q_r - q_{ro} - E_a - q_d \tag{4}$$

where the t is time, q_r, q_{ro} and E_a [L T^{-1}] are the rainfall, runoff, and evapotranspiration rates respectively, and q_d [L T^{-1}] is the drainage rate at the base of the soil column.

All soil zone components are driven by time series of rainfall and potential evapotranspiration, E_p [L T^{-1}].

[1] The UN Food and Agricultural Organisation refer to this as the 'total available water' (Allen et al., 1998). For consistency it's referred to as water available for plant uptake here.

Table 2: Summary of soil zone module components.

ID	Name	Description
1	FAO	Drainage from the base of the soil zone is calculated using a soil water balance method based on a simplification of the algorithm developed by the UN Food and Agricultural Organisation (Allen et al., 1998).
2	NSSS	Includes a near-surface soil store to allow for efficient evaporation of rainfall-wetted soil near the surface (Rushton et al., 2006).
3	SMAP	The Simplified Soil Moisture Accounting Procedure (SMAP) was proposed by Mathias et al. (2015) as a way to emulate the Richards' equation with a relatively simple set of equations that can be solved using a Euler explicit time stepping scheme.

3.1.1 FAO

The FAO component simulates soil moisture as a function of vegetation and soil properties with a saturation-dependant parameterisation of evapotranspiration processes. As the soil moisture deficit increases, it becomes more difficult for vegetation to extract water from the soil matrix. The proportion of Θ_{pu} that can easily be extracted before this point is reached is conceptualised as 'readily available water', Θ_{raw} [L], which is calculated as

$$\Theta_{raw} = p \cdot \Theta_{pu} \tag{5}$$

where p is the depletion factor of the vegetation.

For each time step, all rainfall is assumed to infiltrate into the soil in the first instance ($q_{ro} = 0$). The actual evapotranspiration rate is calculated using a plant stress function that scales the potential evapotranspiration rate according to an intermediate soil moisture deficit, Θ^*_{smd}

$$E_a = \begin{cases} E_p, & \Theta^*_{smd} \leq \Theta_{raw} \\ E_p \left[\dfrac{\Theta_{pu} - \Theta^*_{smd}}{\Theta_{pu} - \Theta_{raw}}\right]^{0.2}, & \Theta_{raw} < \Theta^*_{smd} < \Theta_{pu} \\ 0, & \Theta^*_{smd} \geq \Theta_{pu} \end{cases} \tag{6}$$

where

$$\Theta^*_{smd} = \Theta_{smd_{t-1}} + (E_p - q_r)\Delta t \tag{7}$$

where Δt is the model time step. The intermediate soil moisture deficit is then re-evaluated using the actual evapotranspiration rate

$$\Theta^*_{smd} = \Theta_{smd_{t-1}} + (E_a - q_r)\Delta t \tag{8}$$

When the soil water level exceeds the field capacity ($\Theta^*_{smd} < 0$), any soil water in excess of the evaporative demand of the vegetation becomes excess water, Θ_{exw} [L]

$$\begin{aligned} \Theta_{exw} &= -\Theta^*_{smd}, \quad \Theta_{smd} = 0 \quad \Theta^*_{smd} < 0 \\ \Theta_{exw} &= 0, \quad \Theta_{smd} = \Theta^*_{smd} \quad \Theta^*_{smd} \geq 0 \end{aligned} \tag{9}$$

Any excess water is split between soil drainage and surface runoff instantaneously, q_{ro}

$$q_d = \Theta_{exw} \cdot BFI \quad (10)$$

$$q_{ro} = \Theta_{exw} \cdot (1 - BFI) \quad (11)$$

where BFI [-] is the baseflow index, which defines the average proportion of catchment stream flow that a river receives from groundwater discharge.

Θ may take any value between Θ_{wp} and Θ_{fc}. Therefore, this soil zone component is not expected to replicate periodic saturated soil moisture conditions associated with very wet soils or exceptionally dry soil conditions where only the residual water content remains. Note also that the condition $\theta_{fc} > \theta_{wp}$ must be satisfied. AquiMod automatically substitutes these parameters for one another if this is not satisfied.

Table 3: FAO soil zone component parameters.

Parameter	Description	Recommended range
θ_{fc} (-)	Soil volumetric water content at field capacity	>0 – 1
θ_{wp} (-)	Soil volumetric water content at wilting point	>0 – 1
Z_r (mm)	Maximum root depth of catchment vegetation	100 – 3000
p (-)	Depletion factor of catchment vegetation	>0 – 1
BFI	Catchment baseflow index	>0 – 1

3.1.2 NSSS

The near-surface soil store (NSSS) component uses a different plant stress function to the FAO component and includes an additional near-surface soil store to provide some representation of the vertical distribution of soil moisture in the soil column which can be important for controlling evapotranspiration processes. Specifically, this component allows a dry soil to meet the evaporative demand if the near surface soil is wet from recent rainfall. In this model, a defined proportion of rainfall is assumed to runoff using the baseflow index parameter defined above:

$$q_{ro} = q_r \cdot (1 - BFI) \quad (12)$$

The remaining water infiltrates the soil and a fraction, $FRACSTOR$ of this and any existing near-surface soil water is retained at the near-surface

$$\Theta_{surf_t} = \left[q_r \cdot BFI + \Theta_{surf_{t-1}}\right] \cdot FRACSTOR - E_{a(surf)} \quad (13)$$

where Θ_{surf} is the near-surface soil water level and $E_{a(surf)}$ is actual evaporation from this soil store. At each time step, evapotranspiration commences at the potential rate from the near surface soil store. Any remaining demand is met by deeper soil water. The total actual evapotranspiration from the soil, E_a is calculated as:

$$E_a = \begin{cases} E_p, & \Theta^*_{surf} \geq E_p \\ \Theta^*_{surf} + f_1(\Theta_{\mathrm{smd_{t-1}}}) \cdot \left(E_p - \Theta^*_{surf}\right), & \Theta^*_{surf} < E_p \end{cases} \quad (14)$$

Θ^*_{surf} in an intermediate surface soil storage calculated from eq. 13 where $E_{a(surf)} = 0$. Θ_{smd} is the calculated from eq. 4 and f_1 is the following plant stress function

$$f_1(\Theta_{\text{smd}}) = \begin{cases} 1, & \Theta_{\text{smd}} \leq \Theta_{raw} \\ \dfrac{\Theta_{pu} - \Theta_{\text{smd}}}{\Theta_{pu} - \Theta_{raw}}, & \Theta_{raw} < \Theta_{\text{smd}} < \Theta_{pu} \\ 0, & \Theta_{\text{smd}} \geq \Theta_{pu} \end{cases} \quad (15)$$

Here, Θ_{raw} is calculated following eq. 5.

As with the FAO component, Θ may take any value between Θ_{wp} and Θ_{fc}. Therefore, this soil zone component is not expected to replicate periodic saturated soil moisture conditions associated with very wet soils or exceptionally dry soil conditions where only the residual water content remains. Note also that the condition $\theta_{fc} > \theta_{wp}$ must be satisfied. AquiMod 2 automatically substitutes these parameters for one another if this is not satisfied.

Table 4: NSSS soil zone component parameters.

Parameter	Description	Recommended range
θ_{fc} (-)	Soil volumetric water content at field capacity	>0 – 1
θ_{wp} (-)	Soil volumetric water content at wilting point	>0 – 1
Z_r (mm)	Maximum root depth of catchment vegetation	100 – 3000
$FRACSTOR$ (-)	Fraction of soil water stored at near surface	>0 – 1
p (-)	Depletion factor of catchment vegetation	>0 – 1
BFI	Catchment baseflow index	>0 – 1

3.1.3 SMAP

In this model any rainfall that doesn't exceed a pre-defined soil infiltration capacity q_{ic} [L T^{-1}] is assumed to infiltrate the soil. Any excess rainfall is lost as surface runoff

$$q_{ro} = \begin{cases} q_r - q_{ic}, & q_r \geq q_{ic} \\ 0, & q_r < q_{ic} \end{cases} \quad (16)$$

The drainage rate is approximated using the hydraulic conductivity of the soil, K [L T^{-1}]

$$q_d = K(\hat{S}_e) = K_s \hat{S}_e^{\eta} \left[1 - \left(1 - \hat{S}_e^{1/m}\right)^m\right]^2 \quad (17)$$

where K_s [L T^{-1}] is the saturated hydraulic conductivity and η is an empirical relative permeability exponent. m is calculated from an empirical capillary pressure exponent, γ defined by van Genuchten (1980)

$$m = 1 - {}^{1}/_{\gamma} \quad (18)$$

and the effective saturation, $\hat{S}_e$ is approximated as

$$S_e = \frac{\Theta - \Theta_{wp}}{\Theta_{pu}} \quad (19)$$

where Θ_{pu} and Θ_{wp} are calculated following equations 3 and 4. The actual evapotranspiration is found by scaling the potential evapotranspiration weight according to the soil pressure head, $\hat{\psi}$ [L]

$$E_a = f_2(\hat{\psi})E_p \tag{20}$$

where f_2 is the plant stress function defined by Feddes et al. (1976)

$$f_2(\psi) = \begin{cases} 0, & \hat{\psi} \geq \psi_a \\ 1, & \psi_a > \hat{\psi} > \psi_d \\ 1 - \dfrac{\hat{\psi} - \psi_d}{\psi_w - \psi_d}, & \psi_d \geq \hat{\psi} \geq \psi_w \\ 0, & \hat{\psi} < \psi_w \end{cases} \tag{21}$$

Following Feddes et al. (1976), the critical pressure heads associated with soil water-limited evapotranspiration (ψ_d) and plant wilting (ψ_w) are set to -4 and -150 m respectively. The pressure head associated with anaerobiosis (ψ_a) is reserved as a calibration parameter. The pressure head [L] is approximated using the effective saturation

$$\hat{\psi} = -\beta^{-1}\left(\hat{S}_e^{-1/m} - 1\right)^{1/\gamma} \tag{22}$$

where β is the reciprocal of air-entry pressure [L^{-1}].

As with the other soil zone components, Θ may take any value between Θ_{wp} and Θ_{fc}. Therefore, this soil zone component is not expected to replicate saturated soil moisture conditions associated with very wet soils or very dry soil conditions where only the residual water content remains. Note also that the condition $\theta_{fc} > \theta_{wp}$ must be satisfied. AquiMod 2 automatically substitutes these parameters for one another if this is not satisfied.

Table 5: SMAP soil zone component parameters.

Parameter	Description	Recommended range
θ_{fc} (-)	Soil volumetric water content at field capacity	>0 – 1
θ_{wp} (-)	Soil volumetric water content at wilting point	>0 – 1
Z_r (mm)	Maximum root depth of catchment vegetation	100 – 3000
q_{ic} (mm d^{-1})	Soil infiltration capacity	10 – 100
K_s (m d^{-1})	Depletion factor of catchment vegetation	0.1 – 10
η (-)	Relative permeability exponent	-10 – 1
γ (-)	Capillary pressure exponent	1 – 3
β (mm^{-1})	Reciprocal of air-entry pressure	500 – 4000
ψ_a(mm)	Pressure head associated with anaerobiosis	-5e-5 – 0

3.2 UNSATURATED ZONE MODULE

There is one unsaturated zone component available in the AquiMod software (Table 6).

Table 6: Summary of unsaturated zone module components.

ID	Name	Description
1	Weibull	Drainage from the soil is attenuated through the unsaturated zone using a Weibull distribution transfer function.

3.2.1 Weibull

Recharge, q_{rech} [L T^{-1}] is calculated as the weighted sum of soil draining over the preceding n time steps:

$$q_{rech_t} = \omega \sum_{x=1}^{n} f_2(x) \cdot q_{d_{t-x+1}} \tag{23}$$

where f_2 is a two-parameter Weibull probability density function

$$f_2(x;\lambda,k) = \begin{cases} \frac{k}{\lambda}\left(\frac{x}{\lambda}\right)^{k-1} e^{-(x/\lambda)^k} & x \geq 0 \\ 0 & x < 0 \end{cases} \tag{24}$$

and where ω is a scaling parameter such that the discrete integral is equal to unity. k > 0 is the shape parameter and λ > 0 is the scale parameter of the distribution. The λ parameter primarily controls the location of the peak in the probability density function while k controls the density of the function around the peak (Figure 4). The Weibull function can represent exponentially increasing, exponentially decreasing, and positively and negatively skewed distributions. It is used because it allows the exploration of different distributions, whilst being smooth, which is more physically justifiable than randomly selected monthly weights.

Note, the ω and n parameters are both determined by the AquiMod 2 code to optimise the performance of the model so these do not need to be specified by the user.

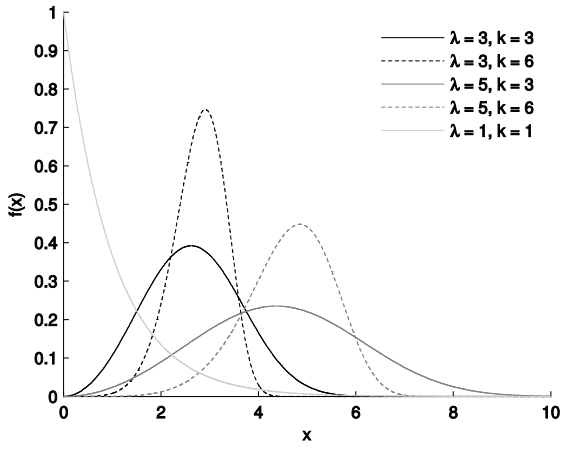

Figure 4: Probability distribution function of the Weibull distribution using different λ and k combinations.

Table 7: Weibull unsaturated zone component parameters.

Parameter	Description	Recommended range
k (-)	Weibull shape parameter	1-7
λ (-)	Weibull scale parameter	>0

3.3 SATURATED ZONE MODULE

There are eight saturated zone components available in the AquiMod 2 software (Table 8).

Table 8: Summary of saturated zone module components.

ID	Name	Description
1	Q3K3S1	A three-layer aquifer representation, each of variable thickness and permeability.
2	Q2K2S1	A two-layer aquifer representation, each of variable thickness and permeability.
3	Q1K1S1	A single layer aquifer representation.
4	Q1T1S1	A confined aquifer representation with a fixed transmissivity.
5	VKD	An aquifer with a 'cocktail glass' representation of the change in hydraulic conductivity with depth.
6	Q3K3S3	A three-layer aquifer representation, each of variable thickness, permeability, and storage coefficient.
7	Q2K2S2	A two-layer aquifer representation, each of variable thickness, permeability, and storage coefficient.
8	SA1D	A semi-analytical solution to the 1D groundwater flow equation proposed by Park and Parker (2008).

3.3.1 Q3K3S1

This component represents flow in the saturated zone by a rectangular block of aquifer with dimensions Δx and Δy denoting its length and width [L] respectively. A mass balance calculation is performed at each time step to calculate the new groundwater head

$$q_{rech}\Delta x\Delta y - Q - ABS = S\Delta x\Delta y\frac{dh}{dt} \quad (25)$$

where Q is the total groundwater discharge [$L^3 T^{-1}$], ABS [$L^3 T^{-1}$] is any additional abstraction, S is the storage coefficient and dh is the change in groundwater head [L] over time, dt [T].

This component accommodates three layers of variable thickness and permeability (Figure 5). Each layer is independent and has its own discharge outlet. The deepest layer represents groundwater which flows out of the catchment. The two upper outlets are lumped representations of surface discharge points in the catchment including rivers and springs. Both may flow intermittently if the groundwater head falls below the outlet elevation.

The total groundwater discharge is the sum of discharge from all layers in the saturated zone which is calculated using an equation of the form

$$Q = \sum_{i=1}^{m} \frac{T_i \Delta y}{0.5\Delta x} \Delta h_i \tag{26}$$

where i is the layer number for m layers and Δh_i [L] is the difference between the groundwater head and the elevation of the aquifer outlet point. Due to the explicit form of Equation 9 used, the groundwater head at the previous time step, h^* [L] is used

$$\Delta h_i = \begin{cases} h^* - z_i & h^* > z_i \\ 0 & h^* \leq z_i \end{cases} \tag{27}$$

where z_i is the outlet elevation. Transmissivity, T_i [$L^2 T^{-1}$] is a function of the hydraulic conductivity [$L T^{-1}$], K_i, and is calculated using the following piecewise function

$$T_i = \begin{cases} 0 & h^* \leq z_i & i = (1 \ldots m) \\ K_i(h^* - z_i) & z_i < h^* < z_{i+1} & i < m \\ K_i(z_{i+1} - z_i) & h^* \geq z_{i+1} & i < m \\ K_m(h^* - z_m) & h^* > z_m & i = m \end{cases} \tag{28}$$

Using this component, the hydraulic conductivity can be configured to increase or decrease with depth by modifying the K parameters. This may in itself be an important physical characteristic of the study aquifer. For many aquifers the hydraulic conductivity decreases with depth. An additional α parameter can be switched to force this condition. By setting this to 1, regardless of how the three K values are specified, AquiMod will automatically rearrange them to ensure that $K_3 \geq K_2 \geq K_1$. This option is particularly useful when calibrating AquiMod. A worked example of this is given in the tutorial in section 6.1.

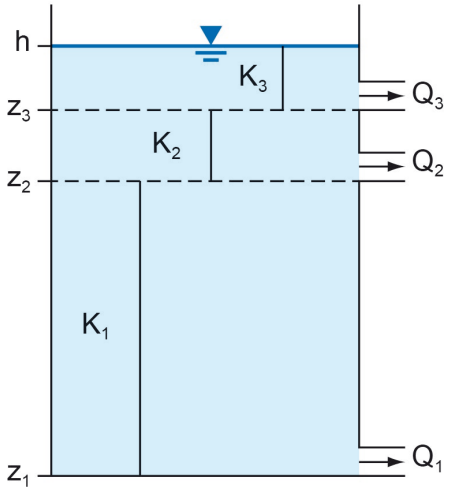

Figure 5: Q3K3S1 saturated zone component.

Table 9: Q3K3S1 saturated zone component parameters.

Parameter	Description	Recommended range
Δx (m)	Catchment length	>0
K_3 (m d^{-1})	Top layer hydraulic conductivity	10^{-5} – 10^{3}
K_2 (m d^{-1})	Middle layer hydraulic conductivity	10^{-5} – 10^{3}
K_1 (m d^{-1})	Bottom layer hydraulic conductivity	10^{-5} – 10^{3}
S (-)	Aquifer storage coefficient	0 – 1
z_3 (m)	Top outlet elevation	-∞ - ∞
z_2 (m)	Middle outlet elevation	-∞ - ∞
z_1 (m)	Bottom outlet elevation	-∞ - ∞
α (-)	Forces $K_3 \geq K_2 \geq K_1$ when set to 1	0,1 (Boolean)

3.3.2 Q2K2S1

This component follows equations 25-28 with only two layers. Each layer is independent and has its own discharge outlet (Figure 6). The deepest layer represents groundwater which flows out of the catchment via subsurface flow paths. The upper outlet is a lumped representation of surface discharge points in the catchment including rivers and springs. It may flow intermittently if the groundwater head falls below the outlet elevation. As with the Q3K3S1 component, the hydraulic conductivity can be forced to increase with elevation by specifying the α parameter.

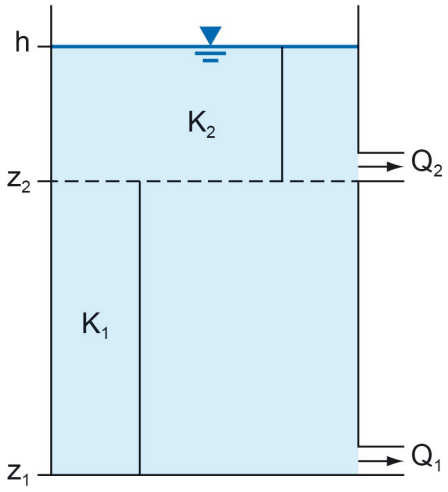

Figure 6: Q2K2S1 saturated zone component.

Table 10: Q2K2S1 saturated zone component parameters.

Parameter	Description	Recommended range
Δx (m)	Catchment length	>0
K_2 (m d^{-1})	Top layer hydraulic conductivity	10^{-5} – 10^{3}
K_1 (m d^{-1})	Bottom layer hydraulic conductivity	10^{-5} – 10^{3}
S (-)	Aquifer storage coefficient	0 – 1
z_2 (m)	Top outlet elevation	-∞ - ∞
z_1 (m)	Bottom outlet elevation	-∞ - ∞
α (-)	Forces the hydraulic conductivity to increase with elevation when set to 1	0,1 (Boolean)

3.3.3 Q1K1S1

This component follows equations 25-28 with only a single and discharge outlet (Figure 7).

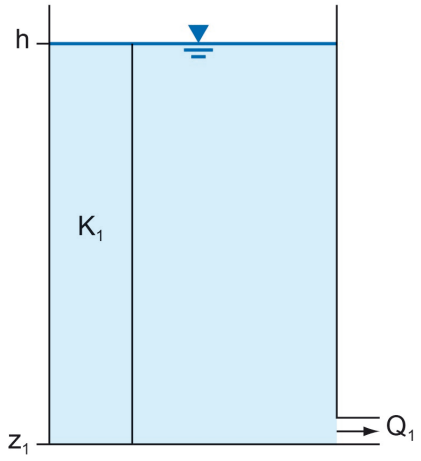

Figure 7: Q1K1S1 saturated zone component.

Table 11: Q1K1S1 saturated zone component parameters.

Parameter	Description	Recommended range
Δx (m)	Catchment length	>0
K_1 (m d^{-1})	Hydraulic conductivity	10^{-5} – 10^{3}
S (-)	Aquifer storage coefficient	0 – 1
z_1 (m)	Outlet elevation	-∞ - ∞

3.3.4 Q1T1S1

Like the Q1K1S1 saturated zone component, this component also employs a single outlet (Figure 8). However, the transmissivity is assumed to be fixed and independent of the hydraulic head, h. This is equivalent to a confined aquifer representation.

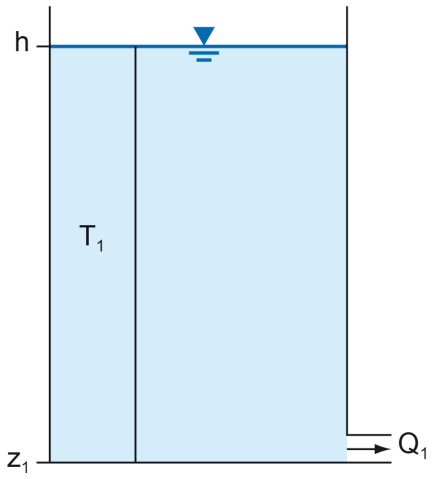

Figure 8: Q1T1S1 saturated zone component.

Table 12: Q1T1S1 saturated zone component parameters.

Parameter	Description	Recommended range
Δx (m)	Catchment length	>0
T_1 (m^2 d^{-1})	Transmissivity	10^{-5} – 10^{3}
S (-)	Aquifer storage coefficient	0 – 1
z_1 (m)	Outlet elevation	-∞ - ∞

3.3.5 VKD

As an alternative to using specified layers and outlets, the user can also implement a variable conductivity with depth (VKD) profile. Here a 'cocktail glass' representation can be employed which has two distinct sections (Figure 9). In the lower section, between the base of the aquifer, z_1 and the elevation of the point of inflection, z_p, the hydraulic conductivity is constant. In the upper section above z_p, the hydraulic conductivity increases linearly with elevation. Subsequently, the transmissivity is calculated as

$$T = K_1(h^* - z_1) + 0.5 \cdot m\left(h^* - z_p\right)^2 \tag{29}$$

where K_1 is the hydraulic conductivity at the base of the aquifer and m is the gradient of the hydraulic conductivity profile above the point of inflection. The total discharge is then calculated as before

$$Q = \frac{T\Delta y}{0.5\Delta x}(h^* - z_1) \tag{30}$$

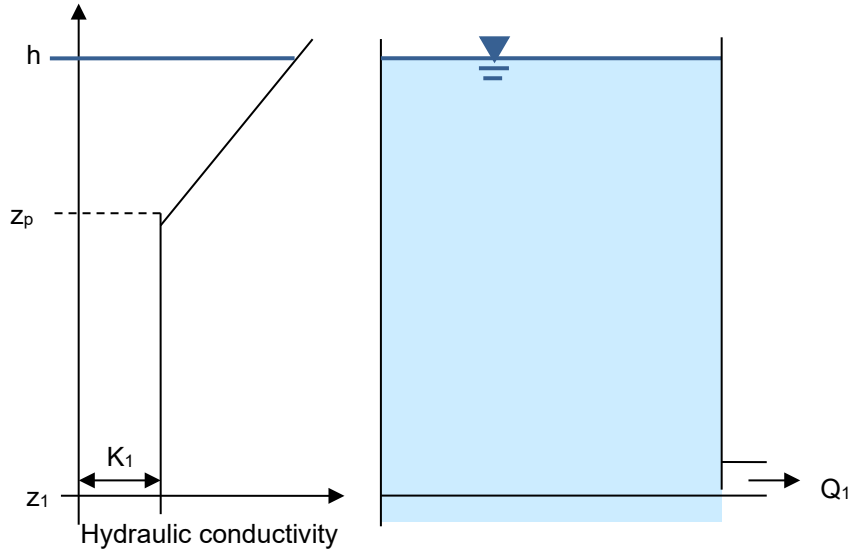

Figure 9: VKD saturated zone component.

Table 13: VKD saturated zone component parameters.

Parameter	Description	Recommended range
Δx (m)	Catchment length	>0
K_1 (m d^{-1})	Hydraulic conductivity at the base of the aquifer	10^{-5} – 10^{3}
m (d^{-1})	Gradient of hydraulic conductivity profile above z_p	0 - 5
S (-)	Aquifer storage coefficient	0 – 1
z_1 (m)	Outlet elevation	-∞ - ∞
z_p (m)	Elevation of hydraulic conductivity inflection	-∞ - ∞

3.3.6 Q3K3S3

This component is identical to the three-layer Q3K3S1 saturated zone component except that the user can specify a unique storage coefficient for each layer. Each layer is independent and has its own discharge outlet. The deepest layer represents groundwater which flows out of the catchment via subsurface flow paths. The two upper outlets are lumped representations of surface discharge points in the catchment including rivers and springs. Both may flow intermittently if the groundwater head falls below the outlet elevation.

Table 14: Q3K3S3 saturated zone component parameters.

Parameter	Description	Recommended range
Δx (m)	Catchment length	>0
K_3 (m d^{-1})	Top layer hydraulic conductivity	10^{-5} – 10^{3}
K_2 (m d^{-1})	Middle layer hydraulic conductivity	10^{-5} – 10^{3}
K_1 (m d^{-1})	Bottom layer hydraulic conductivity	10^{-5} – 10^{3}
S_3 (-)	Top layer storage coefficient	0 – 1
S_2 (-)	Middle layer storage coefficient	0 – 1
S_1 (-)	Bottom layer storage coefficient	0 – 1
z_3 (m)	Top outlet elevation	-∞ - ∞
z_2 (m)	Middle outlet elevation	-∞ - ∞
z_1 (m)	Bottom outlet elevation	-∞ - ∞
α (-)	Forces the hydraulic conductivity to increase with elevation when set to 1	0,1 (Boolean)

3.3.7 Q2K2S2

This component is identical to the two-layer Q2K2S1 saturated zone component except that the user can specify a unique storage coefficient for each layer. Each layer is independent and has its own discharge outlet. The deepest layer represents groundwater which flows out of the catchment via subsurface flow paths. The upper outlet is a lumped representation of surface discharge points in the catchment including rivers and springs. It may flow intermittently if the groundwater head falls below the outlet elevation.

Table 15: Q2K2S2 saturated zone component parameters.

Parameter	Description	Recommended range
Δx (m)	Catchment length	>0
K_2 (m d^{-1})	Top layer hydraulic conductivity	10^{-5} – 10^{3}
K_1 (m d^{-1})	Bottom layer hydraulic conductivity	10^{-5} – 10^{3}
S_2 (-)	Top layer storage coefficient	0 – 1
S_1 (-)	Bottom layer storage coefficient	0 – 1
z_2 (m)	Top outlet elevation	-∞ - ∞
z_1 (m)	Bottom outlet elevation	-∞ - ∞
α (-)	Forces the hydraulic conductivity to increase with elevation when set to 1	0,1 (Boolean)

3.3.8 SA1D

This component is based on a semi-analytical solution to the 1D groundwater flow equation

$$H = H^* e^{k\Delta t} + \left(q_{rech} - \frac{ABS}{\mathrm{A}}\right)\frac{e^{k\Delta t} - 1}{kS} \quad (31)$$

where $H = h - z_1$ is the head [L] above aquifer bottom elevation, z_1. H^* is the head at the previous timestep, k is an aquifer discharge constant [T^{-1}], Δt is the time step, and A is the catchment area. q_{rech} is the recharge from the unsaturated zone [LT^{-1}] and ABS is groundwater pumping [L^3T^{-1}].

Table 16: SA1D saturated zone component parameters.

Parameter	Description	Recommended range
A (m^2)	Catchment area	>0
k (d^{-1})	Aquifer discharge constant	>0
z_1 (m)	Aquifer bottom elevation	-∞ - ∞
S (-)	Storage coefficient	0 – 1

4 Simulation modes

AquiMod 2 has three simulation modes that can be categorised as either calibration or evaluation modes. The calibration modes are used to test different model structures and parameter sets against one another to determine those that are 'good' at capturing the observed dynamics of the system in question (e.g., groundwater level dynamics). These are determined by quantitatively interrogating the models using one or more of the available objective functions. There are two different calibration modes and each are based on different modelling philosophies.

The Monte Carlo mode provides a 'brute force' calibration approach whereby thousands of random parameterisations of AquiMod are applied in quick succession. Depending on the difficulty of the calibration problem, this approach may require a very large sample size to explore the parameter space in detail, which can be computationally expensive. However, it has the advantage that it provides a means to explore model parameter sensitivity and uncertainty easily. Furthermore, the outputs from the Monte Carlo mode can be translated into predictive confidence intervals relatively easily (see tutorials in sections 6.1 and 6.2 for worked examples).

The Shuffled Complex Evolution (SCE-UA) mode uses a global parameter optimisation algorithm to search the parameter space for the 'good' parameterisations automatically. This has shown to be a very versatile and powerful means to finding the global 'optimum' parameter set. However, it was developed on the premise that a global optimum exists (this is often not the case) and does not lend itself to quantifying parameter uncertainty easily.

The evaluation mode allows the user to specify one or more parameter sets for a particular model structure and generate time series of state variables and fluxes simulated by the model. This mode can be used to evaluate the simulation behaviour and the model 'skill' in more detail and undertake bespoke model evaluation outside of AquiMod if required. This mode is also typically used for prediction purposes.

For all simulation modes, the user may choose to quantify the model performance against either groundwater level measurements or measurements of volumetric soil moisture content if these are available.

4.1 OBJECTIVE FUNCTIONS

There are six different objective functions to choose from for model calibration and evaluation (

Table 17). All of them are calculated using the observed (x_o) and modelled (x_m) groundwater levels or volumetric soil moisture content. The first four objective functions evaluate the model performance over the full range of available observations. Objective functions 5 and 6 use the F-SCORE which is a binary classification measure. The F-SCORE evaluates the model's ability to accurately distinguish between periods where the state variable is above or below a pre-defined threshold (x_{thr}). Here, the simulations are categorised into those that correctly predict above and below the threshold: True Positives (TP) and True Negatives (TN) respectively; and those that incorrectly predict above and below the threshold: False Positives (FP) and False Negatives (FN) respectively. The F-SCORE has been used in the past to assess the model's ability to accurately distinguish periods above and below a pre-defined groundwater flood level for flood forecasting. The Weighted F-SCORE/NSE objective function uses both the F-SCORE and NSE objective functions. The user provides a weight parameter, $\tau \in (0 \leq 1)$ which defines the weight applied to the NSE.

Table 17: Objective functions available in AquiMod 2 for a simulation sequence with n time steps including mathematical description and required user-specified parameters.

ID	Name	Description	Additional parameters
1	Nash-Sutcliffe Efficiency	$NSE = 1 - \frac{\sum_{t=1}^{n}(x_o^t - x_m^t)^2}{\sum_{t=1}^{n}(x_o^t - \overline{x_o})^2}$	-
2	Root Mean Squared Error	$RMSE = \sqrt{\sum_{t=1}^{n}(x_o^t - x_m^t)n^{-1}}$	-
3	Mean Absolute Percentage Error	$MAPE = 100 * \sum_{t=1}^{n}\left\|\frac{(x_o^t - x_m^t)}{x_o^t}\right\| n^{-1}$	-
4	Mean Absolute Error	$MAE = \sum_{t=1}^{n}\left\|\frac{(x_o^t - x_m^t)}{x_o^t}\right\| n^{-1}$	-
5	F-SCORE	$F = \frac{TP}{TP + 0.5(FP + FN)}$	x_{thr}
6	Weighted F-SCORE/NSE	$FNSE = \tau \cdot NSE + (1 - \tau)F$	x_{thr}, τ

4.2 CALIBRATION: MONTE CARLO

In this mode, AquiMod uses an in-built Monte Carlo parameter sampling algorithm that runs AquiMod with MC_n unique parameter sets (up to ~10^7) drawn from a uniform distribution of parameters with user-defined bounds. For each parameter set, the model is run, and the measure of simulation efficiency is calculated by comparing the simulated groundwater level or soil water content time series to available observed data using one of the objective functions. The objective function scores and parameter sets are output in order of simulation efficiency, starting with the most efficient. To limit the output to those models which are deemed useful/acceptable, the user may specify an objective function threshold, MC_{thr} that must be reached (e.g. equalled or exceeded for positively oriented objective functions) for it to be included in the model output. To limit the total number of parameter sets output, the user may also specify an upper limit, MC_{n_max}, of number of runs output by the model.

The specification of suitable MC_{thr} and MC_{n_max} parameter values is important when running large Monte Carlo experiments ($MC_n \geq 10^6$) as organising the runs by simulation efficiency becomes computationally expensive if large numbers of acceptable parameter sets are stored.

To use this simulation mode, the user is required to specify the parameters outlined above and summarised in Table 18 as well as an objective function from the list in

Table 17. The user must also define the 'feasible parameter space'. This is specified as a series of lower and upper bounds for each calibration parameter in the calibration input files. A detailed tutorial for implementing the Monte Carlo calibration approach is given in sections 6.1 and 6.2.

Table 18: Parameters for Monte Carlo calibration mode.

Parameter	Description
MC_n	The number of runs. This can range from 1 to approximately 10^7. The maximum depends on available computer memory.
MC_{thr}	Objective function threshold. This threshold must be reached for a parameter set of a simulation to be considered 'acceptable' for output.
MC_{n_max}	Maximum number of acceptable models: The maximum number of parameter sets that reach the acceptable threshold that will be output.

4.3 CALIBRATION: SHUFFLED COMPLEX EVOLUTION OPTIMISATION

In this mode, AquiMod 2 implements the SCE-UA global optimisation algorithm, which has shown to be a robust and efficient optimisation algorithm for hydrological modelling. The reader is referred to Duan et al. (1993) for a full mathematical description of the method[2]. The SCE-UA algorithm has a number of algorithmic parameters that can be tuned to optimise its performance. A number of these have been hard coded into AquiMod 2 based on the experiments undertaken by Duan et al. (1993). Several though, can be tuned by the user for their application. As with the Monte Carlo approach, the user also needs to specify lower and upper bounds for each calibration parameter as well as an objective function from the list in

Table 17.

In this section, a summary of the five principal steps of the algorithm is provided. The SCE_i symbol is used to denote the algorithmic parameters that can be modified by the user and these are also summarised in Table 19. A detailed tutorial for implementing the SCE-UA calibration approach is given in section 6.4.

Step 1: Generate initial sample of parameter sets

An initial random sample of parameter sets is taken from the feasible parameter space. The objective function is then computed for each parameter set.

Step 2: Rank parameter sets

Sort the parameter sets from most to least efficient according to the objective function.

Step 3: Partition parameter sets into complexes

Partition the parameter sets into SCE_p complexes so that each contains a spread of high to low ranked parameter sets.

[2] Steps six and seven from Duan et al. (1993), section 3.2 are not implemented in AquiMod 2.

Step 4: Evolve each complex

Use the competitive complex evolution (CCE) algorithm to evolve each complex:

- Step 4.1: Take a random subsample (sub-complex) made up of approximately half of the points in the original complex with preference given to high-ranked parameter sets.
- Step 4.2: Determine the centroid of the sub-complex within the feasible parameter space.
- Step 4.3: Establish offspring i.e. a new parameter set that is more efficient than at least one existing parameter set in the sub-complex. This is achieved by 'reflection' and 'contraction' steps (movements in the parameter space made about the sub-complex centroid) or 'mutation' steps (randomly generated parameter sets in the feasible parameter space). The least efficient parameter set in the sub-complex is replaced with the offspring.

The SCE_β parameter specifies the number of times each complex is evolved (step 4). The SCE_α parameter specifies the number of offspring that are generated each time a complex is evolved (step 4.3).

Step 5: Shuffle (re-partition) complexes

Combine all of the evolved complexes into a single sample of parameter sets.

The first two steps are only performed once for a given SCE-UA run. Steps 3-5 constitute an evolution loop. The number of evolution loops are specified by the SCE_n parameter. Note, the sample size in step 1 is set to be $SCE_p(2n+1)$ where n is the number of calibration parameters.

Table 19: Algorithmic parameters for SCE-UA calibration mode.

Parameter	Description	Default value
SCE_n	Number of evolution loops. More loops are more computationally expensive, but more likely to find a global optimum parameter set.	20
SCE_p	Number of complexes. The higher the degree of difficulty of the optimisation problem (e.g., larger number of parameters to optimise), the larger this will need to be to locate the global optimum.	20
SCE_α	The number of offspring that are generated each time a complex is evolved. This must be ≥ 1. As this parameter is increased, the search becomes more strongly biased in favour of local search of the parameter space.	1
SCE_β	The number of times each complex is evolved within each evolution loop.	$2n+1$ where n is the number of calibration parameters

4.4 EVALUATION

When using the evaluation mode, the user is required to specify one or more fixed parameter sets. AquiMod then determines the model efficiency for each of these and generates time series output files for each model component (e.g., groundwater level time series for the saturated zone).

5 Model Files

This section covers the model input files that are used to configure AquiMod 2 as well as the output files generated after running the software. Most text editors are suitable for reading and editing AquiMod files, but it is advantageous to use an editor that displays line numbers as these are used in the example file structures given in this section.

5.1 GENERAL FILE AND FOLDER STRUCTURE

The information required to configure and run AquiMod is stored in a series of text files within a defined folder structure (Figure 10). The Observations.txt file contains the available observational data including rainfall, PET, groundwater level and abstraction rates. The Input.txt file allows the user to specify run options including which module components and simulation mode they wish to use. The files stored in the Calibration and Evaluation folders are used when AquiMod is set to run in these respective modes. The calibration input files are used to set ranges of parameter values to define the feasible parameter space. The evaluation input files are used to set specific parameter sets. Finally, the Output folder is where all model outputs are generated.

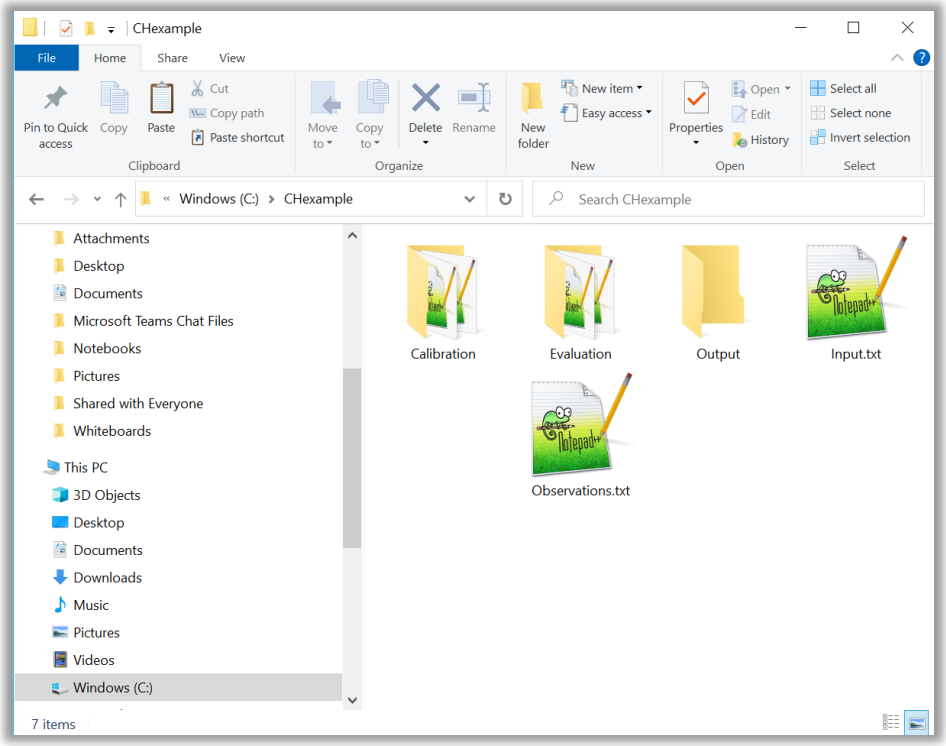

Figure 10: Folder structure of AquiMod.

5.2 INPUT FILES

5.2.1 Observations.txt

Before running AquiMod 2, the user must specify five observation time series along with corresponding date stamps as shown in Figure 11. These data are used to drive AquiMod 2, but the Observations.txt file can also be used to specify other conditions. These are outlined below.

Line number	File contents									Description
1	NUMBER OF OBSERVATIONS									Comment Line
2	365									Number of date-stamped lines of observations in file
3	DAY	MONTH		YEAR	RAIN	PET	SOIL_VWC		GWL	ABS	Headers for columns
4	1	1	2015	0.1	0.5	0.452	15.86	0			[day, month, year, rainfall (mm d^{-1}), PET (mm d^{-1}), soil volumetric water content (-), groundwater level (m), groundwater abstraction rate (m^3 d^{-1})]
5	2	1	2015	0.3	0.45	0.449	-9999	0	s		.
6	3	1	2015	0	0.43	0.413	16.1	0	b		.
.	.										.
.	.										.
368	31	12	2015	1.3	0.36	0.35	15.1	0			.

Figure 11: Example Observations.txt file.

5.2.1.1 DATE STAMPS AND MODEL TIME STEPPING

The model time step is defined by the length of time between each date stamp in the Observations.txt file. The minimum time step is one day, and the time step length can vary throughout the simulation sequence. The model runs from the end of the day specified by the first date stamp (line 4 in Observations.txt) to the end of the day specified by the last date stamp. Accordingly, the total number of time steps is equal to $n - 1$ where n is the number of date-stamped lines of observations specified in the Observations.txt file.

5.2.1.2 RAINFALL AND PET

Continuous time series of rainfall and PET rates in units of mm d^{-1} are required to drive the model. The rainfall and PET on each line of the Observations.txt file should represent the average rainfall rate between the end of the day specified by the date stamp on the previous line to the end of the day specified by the date stamp on the current line. Note that because the model runs from the end of the day specified by the first date stamp (line 4 in Observations.txt), the rainfall and PET rates specified in the first line of observations in the Observations.txt file are not used.

5.2.1.3 SOIL WATER CONTENT

Measurements of volumetric soil water content in the root zone of the soil column are contained in the sixth column. Where measurements are not available, a -9999 value should be entered. These data are used to calculate the specified objective function if calibrating/evaluating against soil moisture data. They may also be used to impose soil moisture conditions (section 5.2.1.7).

5.2.1.4 GROUNDWATER LEVELS

At least one time-stamped measurement of groundwater level in units of metres above a datum is required to run AquiMod, but groundwater level observations do not need to be continuous. Where measurements are not available, a -9999 value should be entered. These data are used to calculate the specified objective function when calibrating or evaluating against groundwater level data. They are also used to initialise the model and may be used to impose groundwater levels (sections 5.2.1.6 and 5.2.1.7).

5.2.1.5 ABSTRACTION RATES

A continuous abstraction rate time series specified in units of m^3 d^{-1} is required. This is subtracted from the saturated zone component during simulation (eq. 25).

5.2.1.6 INITIAL CONDITIONS

AquiMod assumes a dry soil ($\theta = \theta_{wp}$) and unsaturated zone initially. The saturated zone groundwater level is initialised at the beginning of the first time step using the mean of all available groundwater level data in Observations.txt unless an groundwater level observation is specified for the first date-stamped line in Observations.txt (line 4), in which case this is used. Based on the example file in Figure 11, the saturated zone would be initialised with a groundwater level of 15.86 m.

5.2.1.7 IMPOSED GROUNDWATER LEVELS AND SOIL WATER CONTENT

It is possible to impose measurements of groundwater level and soil water content during a simulation. This can be useful when using AquiMod as a forecasting tool to ensure that the initial conditions are as accurate as possible. By imposing measurements, the model discards the simulated value for that time step and uses the observed value instead. This can be done at one or more time steps by placing one of the following characters at the end of the corresponding row(s) in Observations.txt: '*' (impose groundwater level); 's' (impose soil water content); 'b' (impose both groundwater level and soil water content). Based on the example file in Figure 11, the measured volumetric soil water content (0.449) will be imposed on the model simulation at the end of the day on 02/01/2015 and both observations of groundwater level and soil water content will be imposed on the model simulation at the end of the day on 03/02/2015.

5.2.2 Input.txt

The Input.txt file is where the user can specify run options. Each option has a header line and subsequent line where the user can modify the option (Figure 12). These are detailed as follows:

Component IDs

The ID numbers for the desired soil, unsaturated and saturated zone components as indicated in the Tables in section 3. For example, in Figure 12, these have been set to use the SMAP, Weibull, and Q2K2S2 components.

Simulation mode

The simulation mode (as described in Section 4). Either Monte Carlo calibration ('m'), SCE-UA calibration ('s') or evaluation ('e').

Monte Carlo parameters

Used when 'm' is specified as the simulation mode. The parameters include MC_n, MC_{thr}, MC_{n_max} (Table 18) as well as the calibration variable which can be specified as soil water content ('s') or groundwater level ('g').

SCE-UA parameters

Used when 's' is specified as the simulation mode. The parameters include SCE_n, SCE_p, SCE_α, SCE_β (Table 19) as well as the calibration variable, which can be specified as soil water content ('s') or groundwater level ('g').

Evaluation parameters

Used when 'e' is specified as the simulation mode. The parameters include the number of runs as well as the evaluation variable which can be specified as soil water content ('s') or groundwater level ('g').

Objective function and parameters

The objective function ID and associated parameters (

Table 17) used to calculate the model simulation efficiency.

Spin-up period

Since the soil and unsaturated zone components are initiated as dry and the saturated zone may be initiated with an 'average' water storage condition, typically there is an initial wetting-up

or spin-up period where AquiMod may not be able to replicate the observed soil water content and groundwater level time series adequately. Attempting to calibrate a model to observations during this period can result in poor parameter optimisation. To prevent this, the length of this period can be specified as a number of time steps. AquiMod will then ignore this portion of the simulation when calculating the chosen objective function. The length of this period depends on the choice of model structure and parameters. Experience has shown that the memory of the unsaturated zone can be up to ~1 year when the k parameter is small and/or the λ parameter is large. Low diffusivity aquifers where initial groundwater levels are unknown may require multi-year spin-up periods. If in doubt, a spin up period of three years is adequate for most applications.

Write model output files

Here, the user can specify if they wish output files to be written for each model component. When running in one of the calibration modes, a single file is output for each component regardless of the number of runs. In evaluation mode, a separate file is output for each model component and for each model run which can lead to slow runtime when running lots of models. Only switching on the outputs from those components of interest can help to speed up runtime.

Line number	File contents	Description
1	Component IDs	Comment Line
2	3 1 7	Module component selection [Soil, Unsat., Sat.]
3		Blank
4	Simulation mode	Comment Line
5	e	Simulation mode
		m = Monte Carlo calibration
		s = SCE-UA calibration
		e = evaluation
6		Blank
7	Monte Carlo parameters	Comment Line
8	1e4 0.5 1e2 s	[MC_n, MC_{thr}, $MC_{n\ max}$, calibration variable] where calibration variable is:
		s = soil water content
		g = groundwater level
		See Table 18 for parameter details
9		Blank
10	SCE-UA parameters	Comment Line
11	100 50 -1 -1 g	[SCE_n, SCE_p, SCE_α, SCE_β, calibration variable] where calibration variable is:
		s = soil water content
		g = groundwater level
		See Table 19 for parameter details
12		Blank
13	Evaluation parameters	Comment Line
14	1 g	[Number of runs, evaluation variable] where evaluation variable is:
		s = soil water content
		g = groundwater level
15		Blank
16	Objective function and parameters	Comment Line
17	1	[Objective function ID, objective function parameters …] see Table 17 for objective function parameters
18		Blank
19	Spin-up period	Comment Line
20	365	Spin up period (number of time steps) over which objective function will not be calculated.
21		Blank
22	Write model output files	Comment Line
23	Y Y Y	Switch for writing output files [Soil, Unsat., Sat.]
		Y = yes write output file
		N = no do not write output file

Figure 12: Example Input.txt file.

5.2.3 Calibration input files

When running in one of the calibration modes, a separate input file for each module component (soil, unsaturated and saturated zone) must be configured in the Calibration folder. These files

specify the feasible parameter space from which the parameter sets can be sampled. The same calibration input files are used for the Monte Carlo and SCE-UA calibration modes. The file naming convention is *_calib.txt where the asterisk should be replaced by the component name. An example of the FAO_calib.txt calibration input file is given in Figure 13. All calibration input files use the same general structure whereby each component parameter is listed along with two numerical values which specify the lower and upper limit of the feasible parameter space. Also note that parameters can be fixed simply by specifying the same minimum and maximum values, as has been done for the field capacity (θ_{fc}) parameter in Figure 13.

Line number	File contents	Description
1	theta_fc(-)	Comment Line
2	0.4 0.4	Minimum and maximum value
3		Blank
4	theta_wp(-)	Comment Line
5	0.1 0.2	Minimum and maximum value
6		Blank
7	Z_r(mm)	Comment Line
8	100.0 3000.0	Minimum and maximum value
9		Blank
10	p(-)	Comment Line
11	0.1 0.9	Minimum and maximum value
12		Blank
13	BFI(-)	Comment Line
14	0.1 0.99	Minimum and maximum value

Figure 13: Example of the FAO_calib.txt calibration input file format. The field capacity (line 2) is fixed.

5.2.4 Evaluation input files

When running in evaluation mode, a separate input file for each module component (soil, unsaturated and saturated zone) must be configured in the Evaluation folder. These files specify one or more parameter sets where each parameter set is used in turn to run AquiMod once. The file naming convention is *_eval.txt where the asterisk should be replaced by the component name. Figure 14 provides an example of the FAO_eval.txt file. Here two parameter sets are defined.

Line number	File text					Description
1	theta_fc(-)	theta_wp(-)	Z_r(mm)	p(-)	BFI(-)	Header Line
2	0.456503	0.2	167.739	0.1	0.454875	Parameter values (run 1)
3	0.425925	0.188565	177.264	0.218436	0.843572	Parameter values (run 2)

Figure 14: Example of the FAO_eval.txt calibration input file format.

5.3 TEMPLATE CALIBRATION AND EVALUATION INPUT FILES

The structure of the calibration and evaluation input files varies depending on which module components have been specified in Input.txt. AquiMod 2 automatically generates template calibration or evaluation input files when the user fails to them for any module component. The use of this functionality is recommended when switching to a new module component as this will help to ensure that the structures of the input files are correct (see the tutorial in section 6.3 for a worked example of this).

5.4 OUTPUT FILES

After executing the AquiMod software, a series of output text files will be generated in the Output folder (the number of files generated depends on the user specifications in Input.txt). All output files use the '.out' file extension.

5.4.1 Calibration output files

When running AquiMod in one of the calibration modes, and where the output file switches in the input.txt file have been set to 'Y', a single output file for these module components will be generated. These files follow the naming convention *_calib.out where the asterisk is replaced by the component name and contain the parameter sets of the models output from the calibration run. An example Weibull_calib.out file is shown in Figure 15.

For the Monte Carlo calibration mode, only the most efficient MC_{n_max} parameter sets that meet the acceptable model threshold are output. They are ordered from most to least efficient.

For the SCE-UA calibration mode, the output parameter sets summarise the search for (evolution of) the global optimal as the SCE-UA algorithm iterates through the SCE_n evolution loops. Specifically, the output files list one parameter set for each of the SCE_n evolution loops. Each parameter set represents the most efficient of the sample of parameter sets for that evolution loop. They are listed in reverse order, starting from the final evolution loop to the first. It is, therefore, possible to analyse how the optimal parameterisation of the model evolved from the initial sample (last line in the output file) to the identified global optimum after the final evolution loop (line 2 in the output file).

Note that the file structures of the calibration output files are identical to those of the evaluation input files. This allows for easy transfer between calibration and evaluation modes (see tutorial in section 6.2 for worked example of this).

Line number	File contents				Description
1	k(-)	lambda(-)	n(timesteps)		Header Line
2	2.78	2.43	6		Parameter values
3	4.43	2.10	6		.
4	6.49	1.64	6		.
5	3.12	2.06	6		.

Figure 15: Example of Weibull_calib.out file.

In conjunction with the module component output files, a fit_calib.out file is also produced (Figure 16) which lists the corresponding objective function scores for the parameter sets listed in the module component output files.

Line number	File contents	Description
1	ObjectiveFunction	Header Line
2	0.913	Objective function score
3	0.912	.
4	0.908	.
5	0.907	.

Figure 16: Example of fit_calib.out file produced by AquiMod using the NSE objective function.

5.4.2 Evaluation output files

When running AquiMod in evaluation mode, and where the output file switches in the input.txt file have been set to 'Y', a single time series output file for each module component and for each parameter set specified in the *_eval.txt files will be produced. These files follow the naming convention *[1]_TimeSeries*[2].out where *[1] is the component name and *[2] is the model run number. An example of the Q3K3S1 output file for parameter set 1 is shown in Figure 17. Note that the output variables include the simulated discharges from the three outlets and the groundwater level time series. For more information on the output variables produced for each module component see Appendix 1.

A corresponding fit_eval.out file is also produced which returns the objective function score for each parameter set. The structure of this file is identical to that for a calibration run (Figure 16).

Line number	File contents							Description
1	Day	Month	Year	Q3(m3/d)	Q2(m3/d)	Q1(m3/d)	GWL(m)	Header Line
2	31	1	1961	0	0	0	70.665	Variable values
3	28	2	1961	4.82748	5.21203	0.248902	61.1048	.
4	31	3	1961	0.893412	4.06564	0.219899	55.6219	.
5	30	4	1961	0.0516189	3.40817	0.203265	53.9034	.
6	31	5	1961	4.61944e-006	3.20209	0.198052	50.2362	.
.	.							.
.	.							.

Figure 17: Example of Q3K3S1_TimeSeries1.out from an evaluation run.

6 Tutorials

This section provides a series of step-by-step tutorials that can be used to familiarise yourself with the AquiMod 2 software. All tutorials use the models from the CHexample or CFexample folders. If you do not have these already, follow the instructions in section 2.

6.1 HOW TO PERFORM A MONTE CARLO CALIBRATION RUN

This tutorial provides instructions to calibrate an AquiMod 2 model for an observation borehole catchment in the United Kingdom using the Monte Carlo calibration method. You will configure the Observations.txt and Input.txt files and learn about the calibration input files. You will then run a Monte Carlo calibration experiment and examine the model outputs.

6.1.1 The Chilgrove House observation borehole

The Chilgrove House observation borehole is in the Cretaceous Chalk aquifer in the south of the United Kingdom (Figure 18). It has groundwater level records from 1836 and is one of the longest groundwater level time series in the world. Situated in the unconfined Seaford Chalk formation, the hydrograph displays a typical sinusoidal response generated by the seasonal recharge signal typical of unconfined aquifers in the UK. More information on the Chilgrove House observation borehole can be found on the British Geological Survey website at https://www2.bgs.ac.uk/groundwater/datainfo/levels/sites/ChilgroveHouse.html. In this tutorial, you will focus on a monthly 45-year time series of groundwater level data between January 1961 and December 2005 over which reliable rainfall and PET estimates are also available (Figure 19). Monthly measurements of groundwater level, rainfall and PET have been derived from the Enhanced Future Flows and Groundwater (eFLaG) dataset (Hannaford et al., 2022b).

All data for this tutorial can be found in the CHexample folder in the download package.

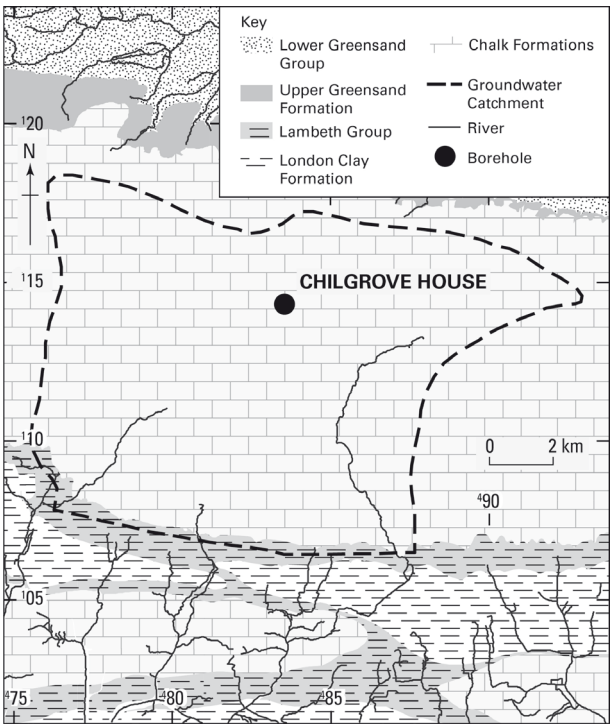

Figure 18: Location of Chilgrove House observation borehole with geological setting and nearby river network. Figure taken from Mackay et al. (2014).

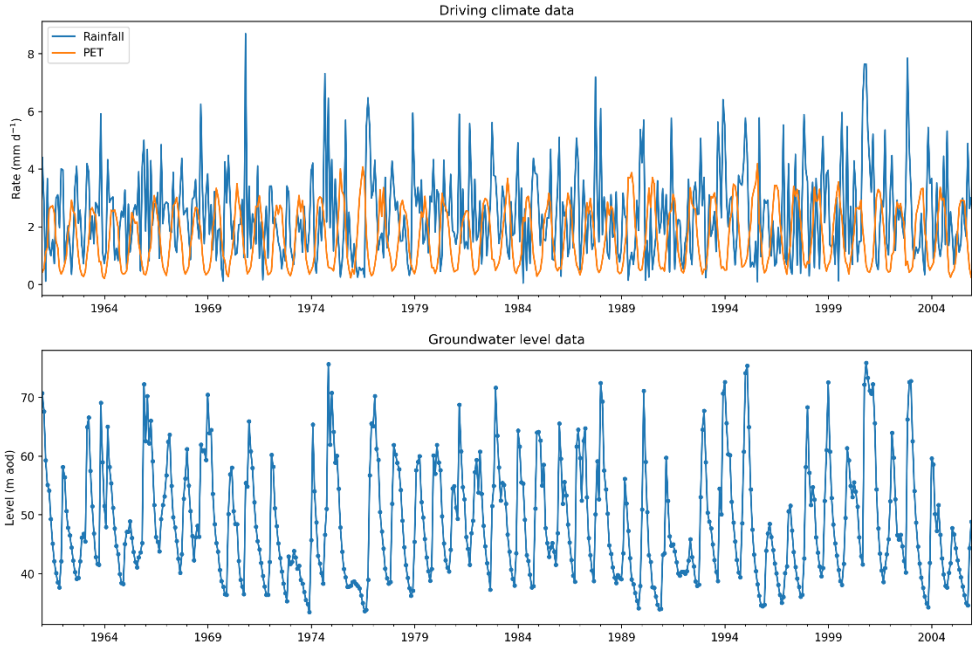

Figure 19: Observed monthly rainfall and PET (top), and groundwater level data (bottom) for the Chilgrove House observation borehole catchment. Contains data supplied by UK Centre for Ecology & Hydrology (Hannaford et al. 2022b).

6.1.2 Observations.txt

First you will calibrate the model against the first half of observed groundwater level data between January 1961 and June 1983. This half of the data can be found in ObsCalib.txt. **Copy and paste this into Observations.txt**. Note that there is no significant groundwater abstraction in the catchment, and as such these rates have been set to zero. Also note that the date stamps show that the model will run on a monthly time step.

6.1.3 Input.txt

Next, you will configure the Input.txt file as shown in Figure 20. Open this file in a text editor. Going through each option in order:

- **Component IDs** – you will use the FAO, Weibull and Q3K3S1 module components so these should all be set to 1.
- **Simulation mode** – this should be set to 'm' to run in Monte Carlo calibration mode.
- **Monte Carlo parameters** – Refer back to Figure 12, line 8 to remind yourself of the Monte Carlo parameters:
    - **Number of runs** – for this tutorial you will run the model 100,000 times in order to find the most efficient parameter sets.
    - **Acceptable model threshold** – deciding upon a suitable value for this will depend on the type of application and personal preferences. For this tutorial we're going to use the NSE with an arbitrary threshold of 0.7.
    - **Maximum number of acceptable models** – again, defining this value is likely to depend on the proposed application. For this tutorial, you will only consider up to the most efficient 1000 models.
    - **Calibration variable** – you're going to calibrate the model against measurements of groundwater level so this should be set to 'g'.
- **SCE-UA parameters** – These parameters have no impact on the Monte Carlo simulation mode and so can be left as they are.
- **Evaluation parameters** – These parameters have no impact on the Monte Carlo simulation mode and so can be left as they are.

Objective function and parameters – Here you will use the Nash Sutcliffe Efficiency. If you refer to

- Table 17, you will see that it has the ID '1' and has no parameters, so you should simply insert a '1' here.
- **Spin-up period** – a spin-up period of 6 time steps (months) is sufficient for this observation borehole catchment.
- **Write model output files** – in calibration mode, the output files will contain the parameter sets of the most efficient Monte Carlo simulations. You will need this information later, so set all of these to 'Y'.

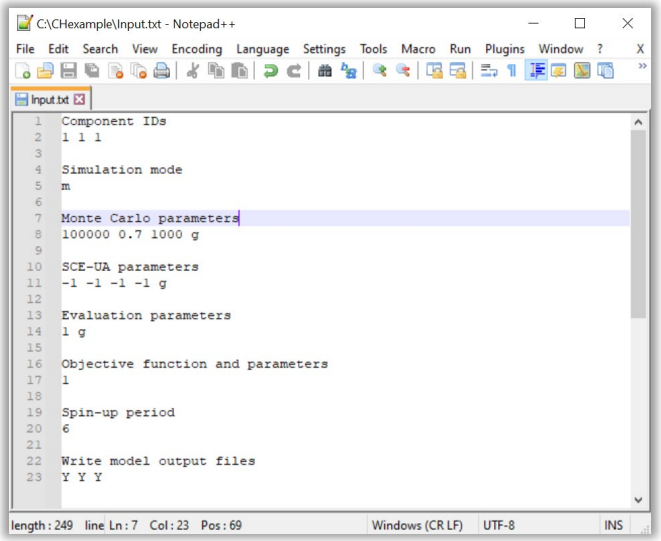

Figure 20: Configured Input.txt file for the Chilgrove House calibration run.

6.1.4 Calibration input files

For this example, the calibration input files have been pre-configured so that a total of 8 of the 16 parameters will be calibrated, while the remainder are fixed. This was determined based on the availability of catchment data.

Open the FAO_calib.txt file located in the Calibration folder. The field capacity (θ_{fc}), wilting point (θ_{wp}) and baseflow index (BFI) parameters have been fixed based on known catchment information obtained from a soil database of the United Kingdom (Boorman et al., 1995) while the maximum root depth (Z_r) and depletion factor (p) are to be randomly sampled between specified ranges.

Next, **open the Weibull_calib.txt file**. The Weibull λ parameter range has been determined by analysing the relationship between rainfall and groundwater levels. The λ parameter controls the location of the peak of the Weibull distribution, or in other words the peak recharge response to rainfall-driven soil drainage. A cross-correlation analysis has been performed between monthly rainfall and groundwater levels (Figure 21) that shows a peak correlation at a 1-month lag. Accordingly, the λ range has been set from 0.1 – 3.0. The k parameter range has been set to 1-7 which is a typical range for this distribution parameter.

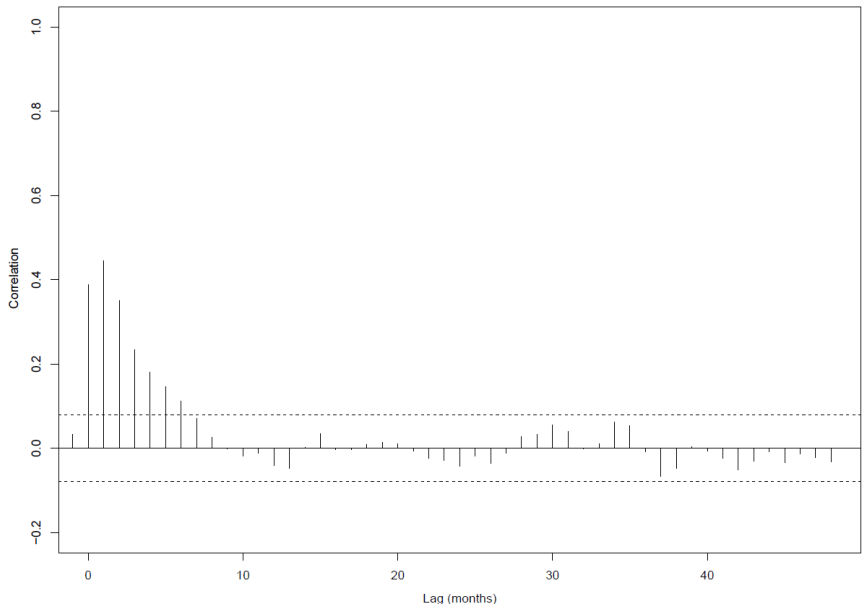

Figure 21: Cross-correlations between rainfall and de-seasonalised groundwater levels.

Finally, **open Q3K3S1_calib.txt**. The aquifer length (Δx) has been fixed to 3000 m which is the approximate length between the borehole and the nearest river in the catchment where the groundwater discharges. The bottom elevation of the aquifer (z_1) has been set based on the known geometry of the Chalk aquifer in this catchment. The second layer outlet elevation (z_2) has also been set. The top layer elevation (z_3) has been kept as a calibration parameter and is free to fluctuate between ground level elevation and the minimum groundwater level on record i.e., within the zone of fluctuation. The storage coefficient (S) and hydraulic conductivity ranges have been set based on known Chalk properties. In this case, the conductivities have been set to decrease with depth as this is a common characteristic of the Chalk aquifer. Since some of the conductivity ranges between layers overlap, some of the random parameter sets sampled by the Monte Carlo routine may, inadvertently, result in hydraulic conductivity profiles that do not monotonically decrease with depth. Accordingly, the α parameter has been set to 1 so that AquiMod automatically arranges the conductivity values so that this condition is satisfied.

6.1.5 Running AquiMod 2 in Monte Carlo calibration mode

Having configured all the required input files, AquiMod 2 is now ready to run. **Run AquiMod 2 in the command prompt** as in section 2.2**.** Notice a slight difference in the output messages for this run compared to the evaluation run conducted in section 2.2 (Figure 22). The first message states that the model is running 100,000 times. If the run time extends beyond 10 seconds, an 'estimated time to finish' message appears which is updated every 10 seconds. Once the runs have completed, a new message appears which states that AquiMod 2 is extracting the best models. Typically, this is instantaneous unless MC_{n_max} is very large in which case this step can become the bottleneck in the overall simulation run time. Finally, AquiMod 2 writes the output files to the Output folder and then displays the total model run time.

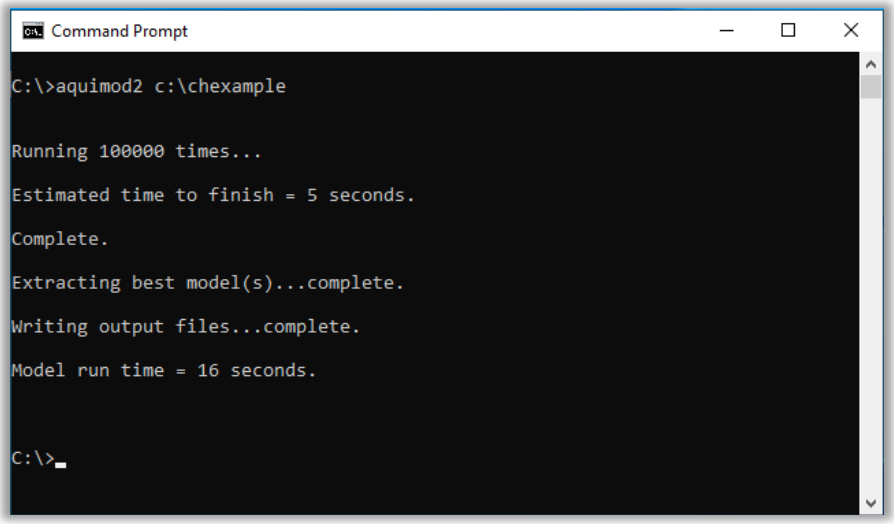

Figure 22: Command prompt view when running AquiMod 2 in the Monte Carlo calibration mode.

6.1.6 Output files

Navigate to the Output folder. AquiMod 2 should have produced a fit_calib.out file as well as a *_calib.out file for each of the three module components. Open the fit_calib.out file to check if any acceptable models have been obtained. The file should be filled with up to 1000 NSE scores. You can use the fit_calib.out file in conjunction with the *_calib.out module component files to assess the identifiability of the parameters. For example, in Figure 23 two 'dotty' plots have been drawn which show that the S parameter is more identifiable (i.e. a particular unique value produces the highest NSE) than the k parameter from the Q3K3S1 saturated zone component and Weibull unsaturated zone component respectively.

If the fit_calib.out file is empty, that means no acceptable models have been obtained. In this case, you may wish to reconsider the criteria for accepting a model, increase the number of runs, adjust the parameter calibration ranges or experiment with different model structures.

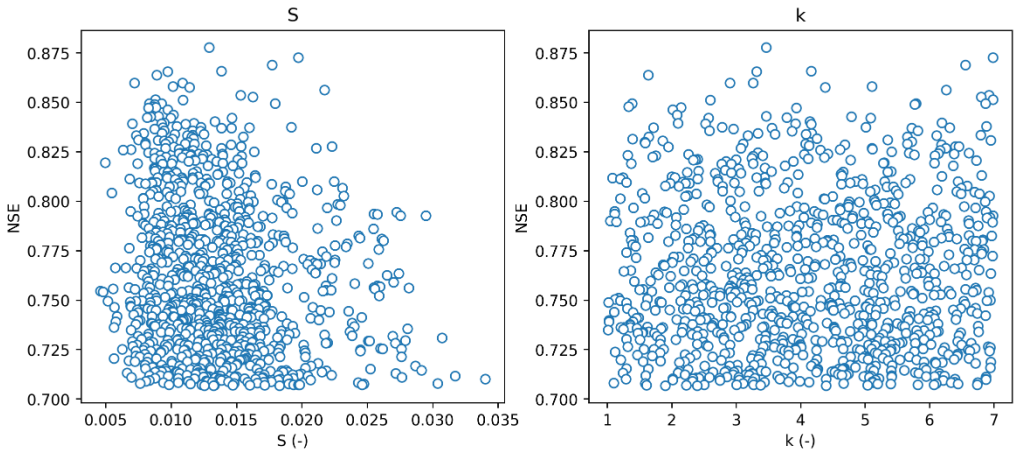

Figure 23: Dotty plots to assess sensitivity of S (left) and k (right) parameters from the Q3K3S1 saturated zone component and Weibull unsaturated zone component respectively. Plots contain 1000 acceptable models obtained from the calibration run.

6.2 HOW TO PERFORM AN EVALUATION RUN

This tutorial provides guidance on how to use AquiMod 2 in the evaluation simulation mode. Here, you are required to specify the parameter sets for one or more prior 'calibration' runs of AquiMod 2. AquiMod generates the simulated time series for the provided parameter sets so that you can evaluate specific model structures and parameter sets by visually comparing the observed and simulated time series.

In this tutorial you will evaluate your newly derived parameter sets from the previous tutorial against all the available data between January 1961 and December 2005.

6.2.1 Observations.txt

First, you need to specify the observed data in the Observations.txt file. These data can be found in ObsEval.txt. Simply **copy and paste** the file contents into Observations.txt. Note that as before we are still running the model on a monthly time step with no abstraction.

6.2.2 Input.txt

Next, you will configure Input.txt as shown in Figure 24. **Open Input.txt in a text editor**. Going through each option in order:

- **Component IDs** – this should remain the same as you will use the same module components.
- **Simulation mode** – set this to 'e' to run in evaluation mode.
- **Monte Carlo parameters** – These parameters have no impact on the evaluation simulation mode and so can be left as they are.
- **SCE-UA parameters** – These parameters have no impact on the evaluation simulation mode and so can be left as they are.
- **Evaluation parameters** – Refer back to Figure 12, line 14 to remind yourself of the evaluation mode parameters:
    - **Number of runs** – Set this to the number of acceptable parameter sets that were obtained from the previous tutorial.
    - **Evaluation variable** – you're going to evaluate the model against measurements of groundwater level so this should be set to 'g'.
- **Objective function and parameters** – This should remain the same.
- **Spin-up period** – This should remain the same.
- **Write model output files** – in evaluation mode, the output files will contain the time series simulations for the acceptable models. In this tutorial you will only assess the groundwater level simulations, so set the first two to 'N' and the last one to 'Y'.

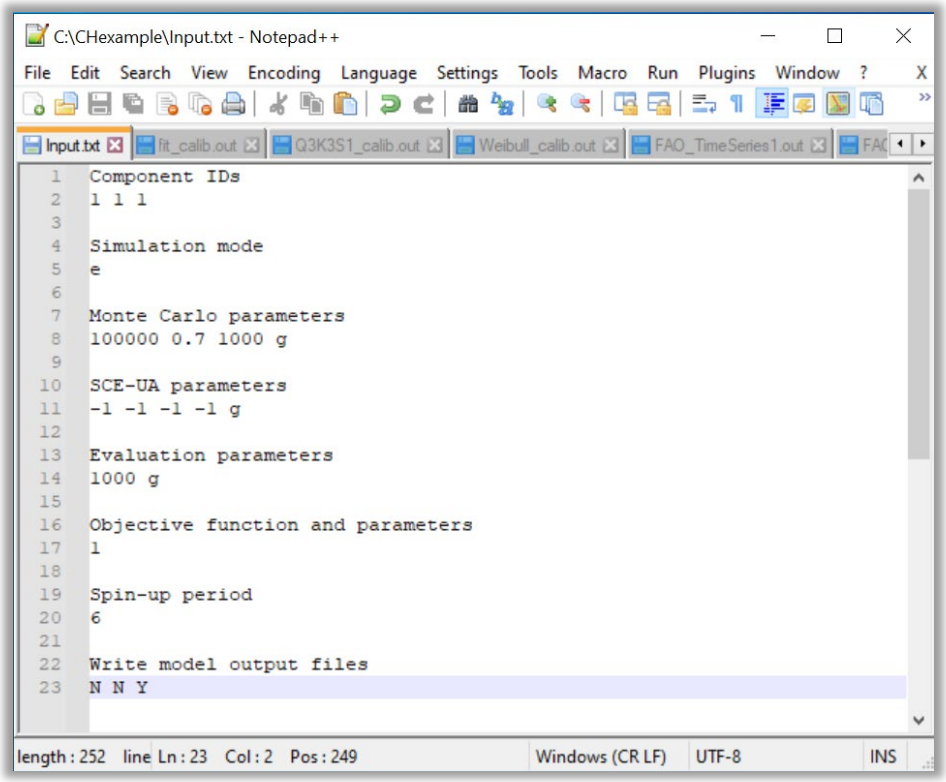

Figure 24: Configured Input.txt file for the Chilgrove House evaluation run.

6.2.3 Evaluation input files

The file structure of the *_eval.txt input files is the same as the output files from the calibration mode. Since you will evaluate the calibrated parameter sets, these files can simply be moved to the Evaluation folder and renamed accordingly. For example, Output\Q3K3S1_calib.out **should be moved and renamed to** Evaluation\Q3K3S1_eval.txt.

6.2.4 Running AquiMod 2 in evaluation mode

Having configured all the required input files, AquiMod 2 is now ready to run as shown in section Figure 25. **Run AquiMod 2 in the command prompt**. This should return similar messages as the calibration run.

Note that the runtime of an evaluation run will typically be longer than a calibration run if any of the ‘Write model output files’ switches in the Input.txt file is set to ‘Y’ as one or more time series files will be written to the Output folder for each run. As such, when performing large numbers of evaluation runs and outputting the results, runtime can increase considerably.

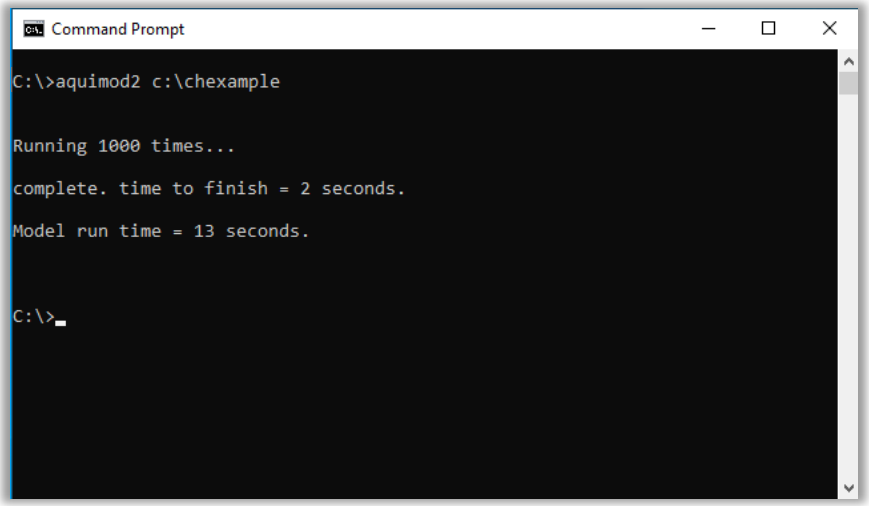

Figure 25: Command prompt view when running AquiMod 2 in evaluation mode.

6.2.5 Output files

After running AquiMod 2 in evaluation mode, it should have produced a fit_eval.out file in the Output folder as well as time series files for each parameter set for the Q3K3S1 module component. Note that the NSE scores recorded in the fit_eval.out file will likely differ to those obtained in the model calibration exercise as you are now evaluating the model against different observation data.

Individual time series can easily be plotted in spreadsheet applications. Plotting the full range of simulations is faster using a scripting language. Figure 26 has been produced using the Python language and shows the 90% confidence interval of the 1000-model simulation against the observations.

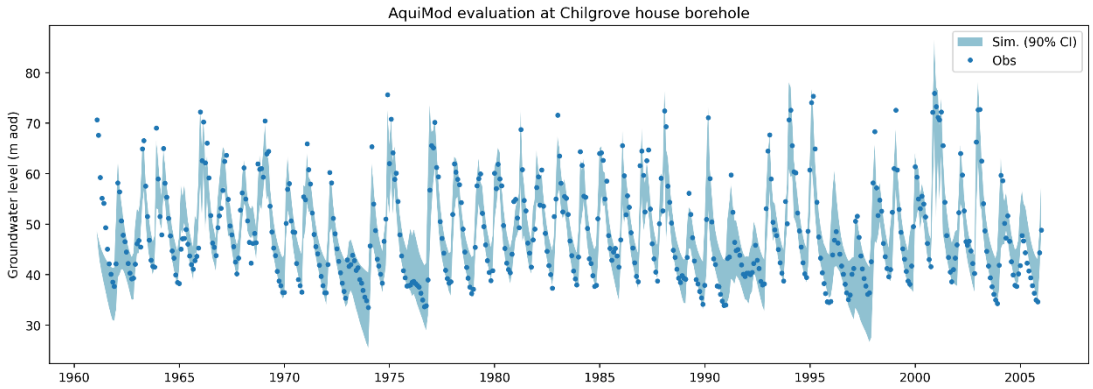

Figure 26: 90% confidence interval of simulations from evaluation runs shown as blue band overlain with observations (dots).

6.3 DEACTIVATING MODULES AND USING OTHER COMPONENTS

You may select any combination of the available module components when using AquiMod. You may also deactivate modules entirely using the ID '0' in Input.txt if you only wish to consider part of the hydrological system. This may be useful if a boundary condition flux is known (e.g., soil drainage) and therefore does not need to be simulated, or if part of the hydrological system is not deemed to be important for a particular application.

If the soil zone is deactivated, evapotranspiration is assumed to be zero and rainfall passes directly to the unsaturated zone as soil drainage. If the unsaturated zone is deactivated, soil drainage is allowed to pass instantaneously to the saturated zone. If both the soil and

unsaturated zone are deactivated, the rainfall input becomes the recharge input to the saturated zone. If the saturated zone is deactivated, groundwater recharge discharges instantaneously out of the model domain.

Experiment with deactivating different modules in the AquiMod 2 structure. You should find that efficient simulations of groundwater levels can still be reproduced without the inclusion of the unsaturated zone component for the Chilgrove House observation borehole.

You may also wish to experiment with using other components. This can be done simply by changing the options in Input.txt and the associated input files. When using new module components you can generate a template calibration or evaluation file, simply by running AquiMod 2 in the associated run mode without the input file(s) present. **Try this now by changing the soil zone component ID from '1' to '2' in the Input.txt file**. By doing so, AquiMod 2 will now try to use the NSSS soil zone component instead of the FAO soil zone component. **Now run AquiMod 2 in the command prompt**.

AquiMod will return an error message to say that the NSSS evaluation input file isn't present and that it has created a template file for you (Figure 27).

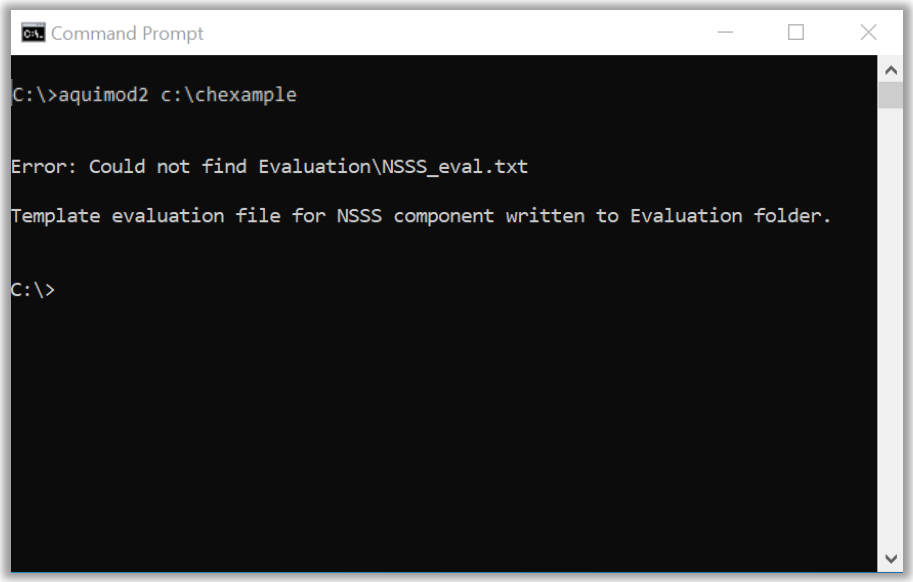

Figure 27: Example output when running AquiMod 2 without one of the required module component input files – in this case, the NSSS evaluation input file.

Now **try changing the simulation mode to 'm' and run AquiMod 2**. You should get a similar message this time, but now the software has built a template calibration input file for the NSSS soil zone component.

6.4 HOW TO PERFORM A SCE-UA CALIBRATION RUN

In this tutorial, you will calibrate a model for the Castle Farm borehole located in the Cretaceous Chalk aquifer in the south-east of the United Kingdom (Figure 28). It has groundwater level records from 1967 and is situated in the unconfined Newhaven Chalk formation. As well as measurements of rainfall, PET and groundwater level data from Hannaford et al. (2022b), nearby measurements of soil water content are also available from the Elmsett cosmic-ray sensing probe which is part of the COSMOS-UK soil moisture monitoring network (Stanley et al., 2021). These data cover the period of August 2016 to November 2018.

In this tutorial you will calibrate three different soil zone module components to the soil water content data using the SCE-UA calibration approach. In the final tutorial in section 6.5 you will calibrate a full AquiMod 2 model (soil, unsaturated and saturated components) to available groundwater level data from 1993 to 2018 using your optimised soil zone models. The

observation data for the site are shown in Figure 29. All data for this tutorial can be found in the CFexample folder in the download package.

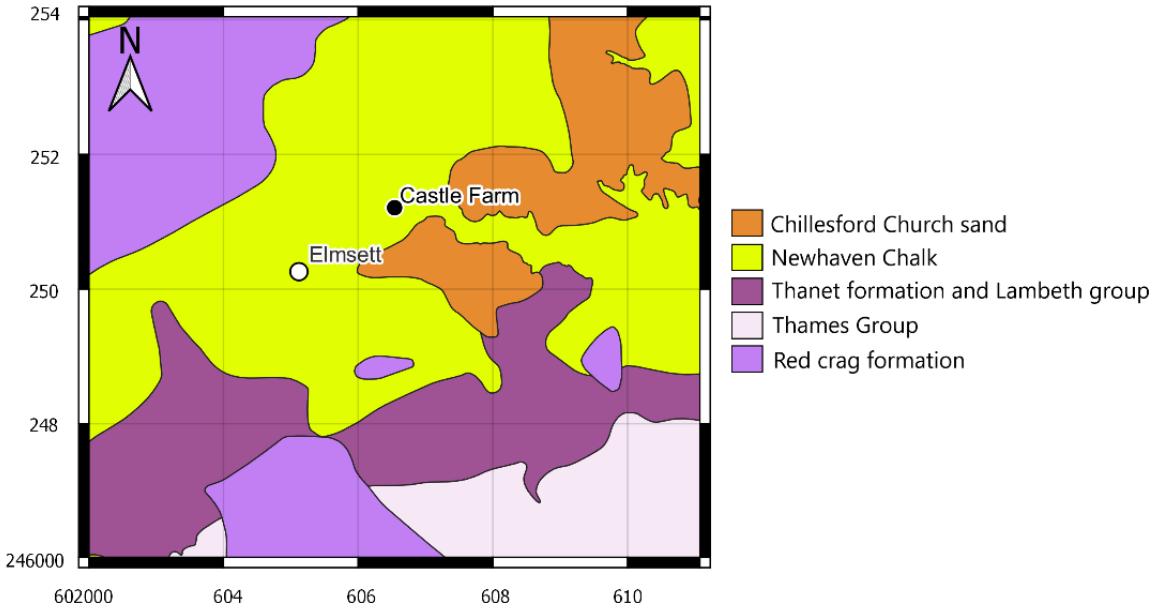

Figure 28: Location of Castle Farm observation borehole and nearby Elmsett soil moisture sensor within its geological setting. Coordinates are in units of metres (British National Grid).

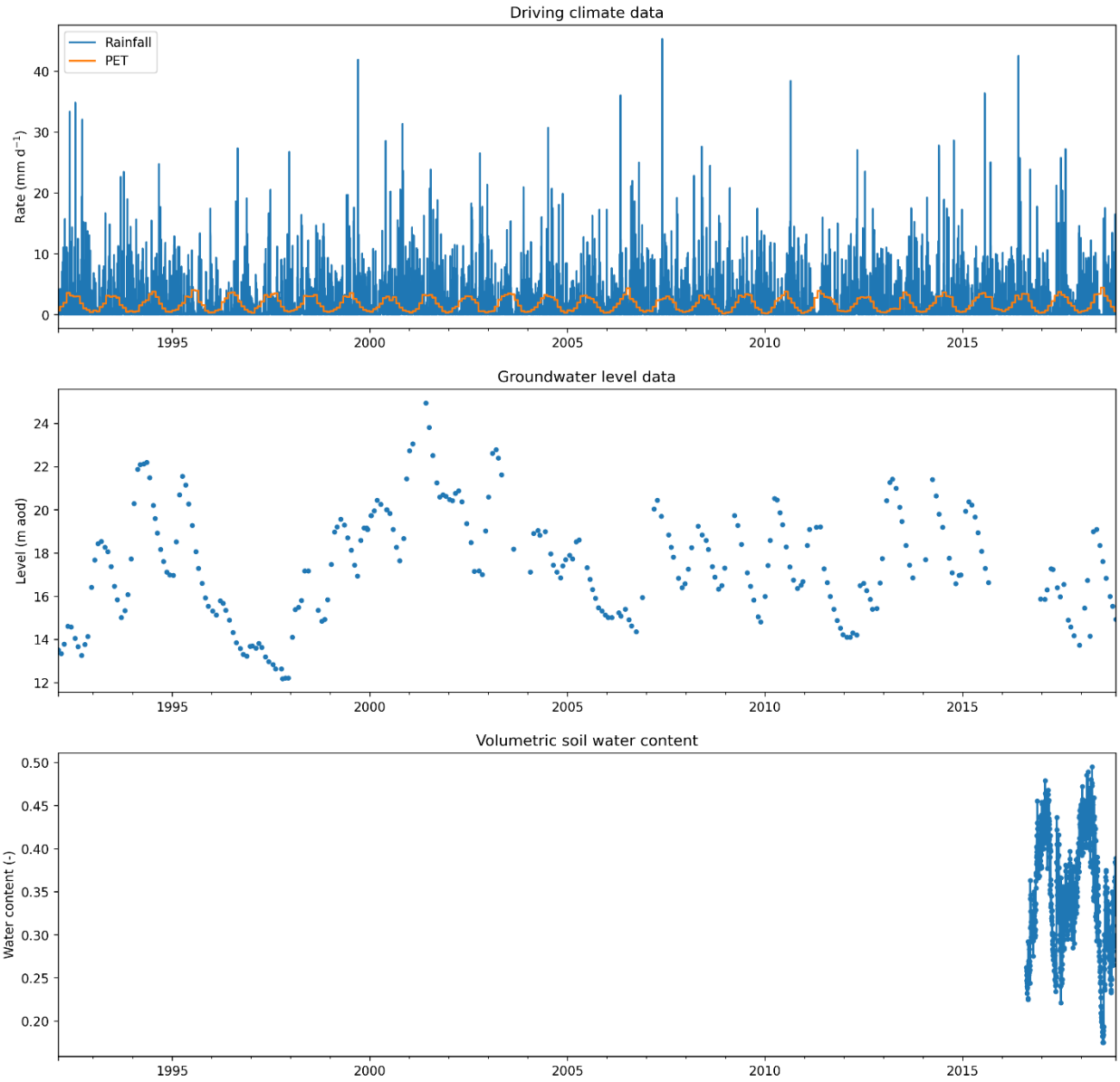

Figure 29: Observed monthly rainfall and PET (top), groundwater level data (middle) and soil water content taken from Elmsett COSMOS-UK station (bottom) for the Castle Farm observation borehole catchment. Contains data supplied by UK Centre for Ecology & Hydrology (Hannaford et al., 2022b; Stanley et al., 2021).

6.4.1 Observations.txt

First you will calibrate the SMAP soil zone component against the observed volumetric soil water content data collected at the Elmsett station. These data can be found in the Observations_for_soil_calib.txt file. **Copy and paste the contents of this file into Observations.txt**. Note that for this study site, the observation data are daily and, therefore, the model will run on a daily time step.

6.4.2 Input.txt

Next, you will configure the Input.txt file as shown in Figure 30. Open this file in a text editor. Going through each option in order:

- **Component IDs** – you will use the SMAP soil zone component only so this should be set to 3. The unsaturated and saturated zone modules should be switched off (set to zero).
- **Simulation mode** – this should be set to ‘s’ to run in SCE-UA calibration mode.

- **Monte Carlo parameters** – These parameters have no impact on the SCE-UA simulation mode and so can be left as they are.
- **SCE-UA parameters** – Refer back to Figure 12, line 11 to remind yourself of the SCE-UA parameters:
    - **Algorithmic parameters** – Start by setting all these parameters (SCE_n, SCE_p, SCE_α, SCE_β) to their default values (Table 19) by setting them to '-1'.
    - **Evaluation variable** – you're going to evaluate the model against observed soil water content data so this should be set to 's'.
- **Evaluation parameters** – These parameters have no impact on the Monte Carlo simulation mode and so can be left as they are.

Objective function and parameters – Here you will use the Nash Sutcliffe Efficiency. If you refer back to

- Table 17, you will see that it has the ID '1' and has no parameters, so you should just insert a '1' here.
- **Spin-up period** – a spin-up period of 365 time steps (days) is sufficient for this catchment.
- **Write model output files** – in calibration mode, the output files will contain the parameter sets of the most efficient parameter set for each SCE-UA evolution loop. You will need this information later, so set the soil zone switch to 'Y'. Note, for this run, because the unsaturated and saturated zone modules are switched off the setting of these to 'Y' or 'N' has no impact on the behaviour of AquiMod.

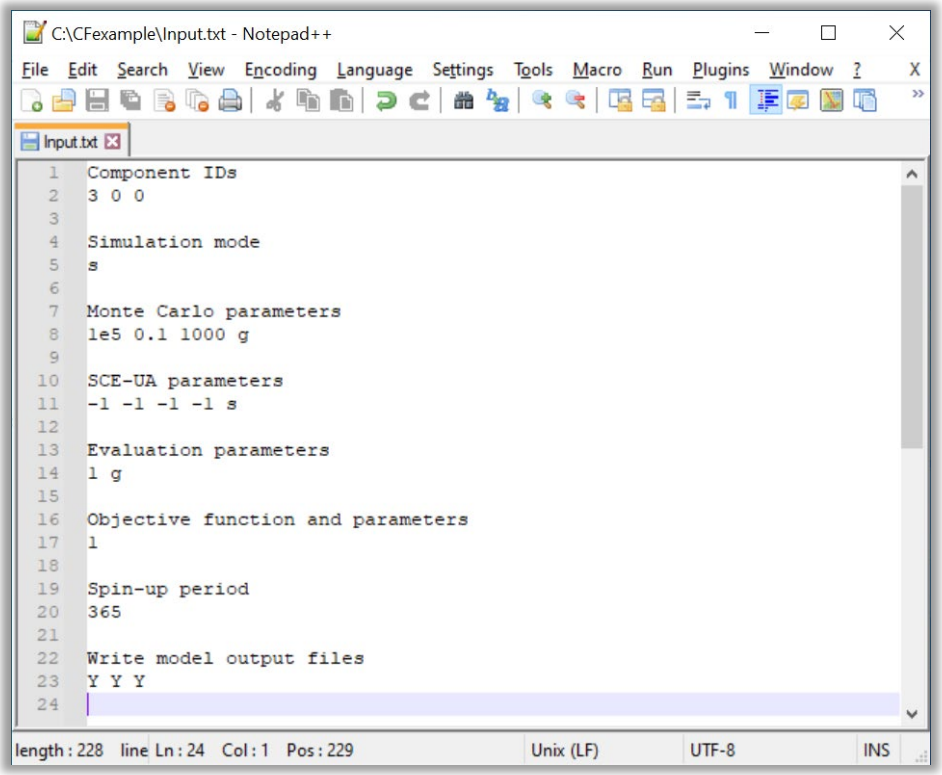

Figure 30: Configured Input.txt file for the Castle Farm SCE-UA calibration run.

6.4.3 Calibration input files

For this example, the calibration input file for the SMAP component has been pre-configured so that all 9 of the parameters will be calibrated. The θ_{fc} and θ_{wp} calibration ranges have been constrained based on local information about the soil to ensure the optimisation makes sense physically. The remaining parameters use typical ranges for vegetation and soil conditions in the UK.

6.4.4 Running AquiMod 2 in SCE-UA calibration mode

Having configured the input files, AquiMod 2 is now ready to run. **Run AquiMod 2 in the command prompt** as in section 2.2**.** Notice the output messages for this run are almost identical to those produced when running a Monte Carlo calibration run except that some additional messages relating to the SCE-UA optimisation are also output (Figure 31). The first message states that the SCE-UA is initialising (steps 1-2 in section 0). Once this has complete, the next message states the total number of evolution loops to complete (steps 3-5 in section 0). Note here that you are using the default value of 20 evolution loops. This is typically the longest part of the SCE-UA approach to run. If the run time extends beyond 10 seconds, an 'estimated time to finish' message appears which is updated every 10 seconds. Once the runs have completed, a new message which states that AquiMod 2 is extracting the best models. Finally, it writes the output files to the Output folder and then states the total model run time.

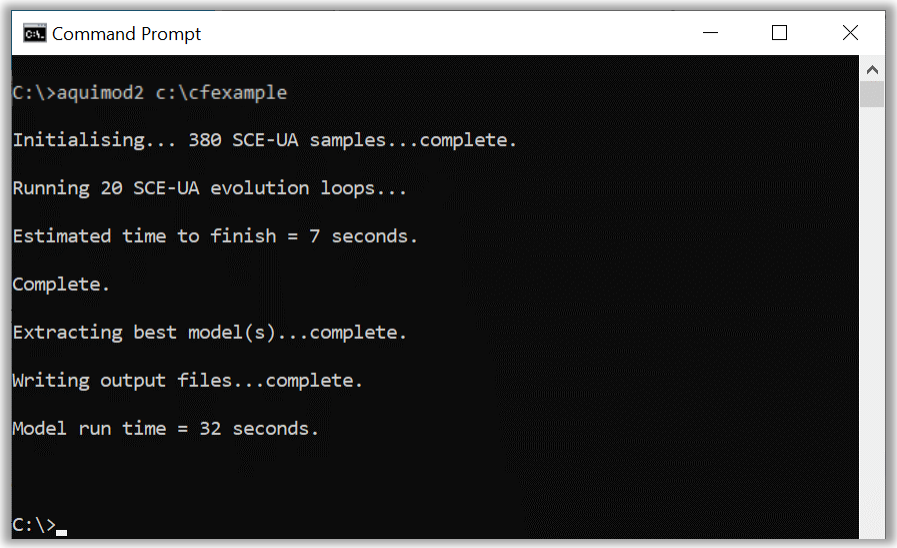

Figure 31: Command prompt view when running AquiMod 2 in the Monte Carlo calibration mode.

6.4.5 Output files

Navigate to the Output folder. AquiMod 2 should have produced a fit_calib.out and SMAP_calib.out file. Open the fit_calib.out file to see the results of the SCE-UA algorithm. The file should have a list of 20 NSE scores – one for each evolution loop. You can see how the fit to the observation data improves with each run. The score at the top corresponds to the overall (global) optimum.

You may want to try doubling or halving the number of evolution loops (SCE_n) and/or the number of complexes (SCE_p) to see what impact it has on the efficiency of the optimised model. Note that doubling one of these parameters will approximately double the runtime but is more likely to result in a parameter set that is at or close to the global optimum.

Figure 32 shows how the NSE score changes as $SCE_n$and SCE_p are changed with values between 1-40. For this calibration problem, a larger SCE_p finds a better 'solution' when using a SCE_n< 10. However, as SCE_n increases, the gain from using a larger SCE_p values are marginal.

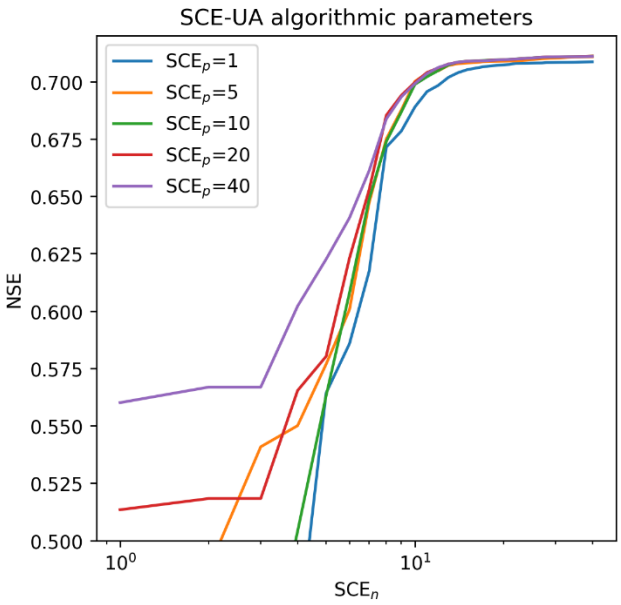

Figure 32: NSE score obtained using the SCE-UA algorithm using different values of $SCE_n$and SCE_p. All data points are based on an average of 10 replicate experiments.

6.4.6 Model evaluation and comparison to other soil zone components.

Once that you are satisfied that you have obtained a solution in or around the global optimum, **configure AquiMod 2 to use this optimal model in evaluation mode to obtain the simulated soil water content time series**. You can refer to section 6.2 if you need to remind yourself how to do this.

Repeat the SCE-UA calibration and evaluation for the other soil zone components (FAO and NSSS). The calibration input files for these modules have been pre-configured for you to do this.

Figure 33a compares the calibrated models obtained using the three different soil zone components against the available observation data. You can see that, in this case, none of the models are able to capture the full soil water content time series and that the deficiencies are different between the models. In this case, the NSSS and SMAP models show almost identical simulation behaviour which broadly capture the soil moisture dynamics except when the volumetric water content falls below 0.3. The FAO model underestimates soil water content for large parts of the observation period. Figure 33b compares the simulated soil drainage (q_d) dynamics of the different models. Here, the timing of drainage episodes is similar across the models, but the magnitude of drainage is highly variable.

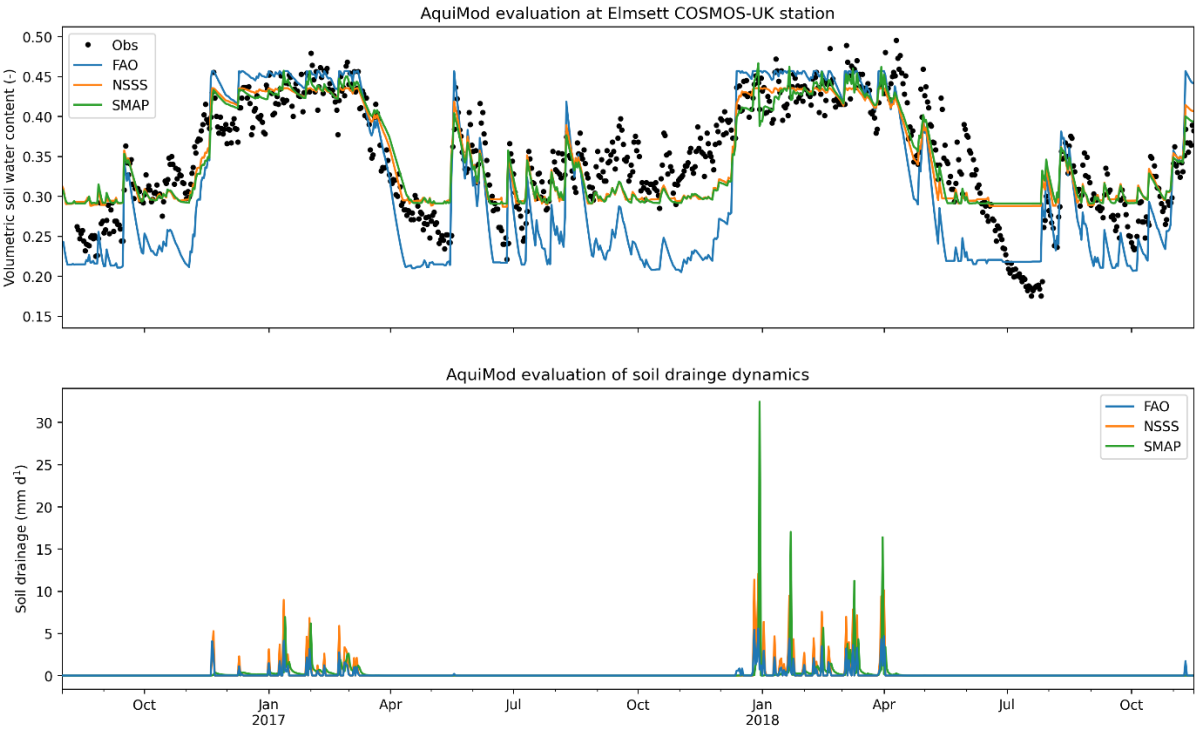

Figure 33: Simulated volumetric soil water content time series from calibrated FAO, NSSS and SMAP soil zone components against observations at Elmsett COSMOS-UK station (top), and simulated soil drainage time series (bottom).

6.5 HOW TO CALIBRATE TO SOIL WATER CONTENT AND GROUNDWATER LEVEL DATA

For this final tutorial, you will take one of your calibrated soil zone models and use it in conjunction with the Weibull unsaturated zone component and the Q2K2S2 saturated zone component so that you can calibrate those components to the available groundwater level data at the Castle Farm borehole. By doing so, you will have built an AquiMod 2 model that has been calibrated to both soil water content and groundwater level data. The intention behind this approach is to provide a more physically consistent model. The examples below assume that you are using your calibrated SMAP soil zone model.

6.5.1 Observations.txt

The observed groundwater level data collected at the Castle Farm borehole can be found in the Observations_for_gw_calib.txt file. **Copy and paste the contents of this file into Observations.txt**.

6.5.2 Input.txt

Next, you will configure the Input.txt file as shown in Figure 34. Open this file in a text editor. Going through each option in order:

- **Component IDs** – you will use the SMAP soil zone component (ID=3) along with the Weibull (ID=1) and Q2K2S2 (ID=7) components.
- **Simulation mode** – this should be set to 's' to run in SCE-UA calibration mode.
- **Monte Carlo parameters** – These parameters have no impact on the SCE-UA simulation mode and so can be left as they are.
- **SCE-UA parameters:**
    - **Algorithmic parameters** – Start by setting all these parameters (SCE_n, SCE_p, SCE_α, SCE_β) to their default values (Table 19) by setting them to '-1'.

    - **Evaluation variable** – you're going to evaluate the model against observed groundwater level data so this should be set to 'g'.
- **Evaluation parameters** – These parameters have no impact on the SCE-UA simulation mode and so can be left as they are.
- **Objective function and parameters** – You will use the Nash Sutcliffe Efficiency again (ID=1).
- **Spin-up period** – keep the spin-up period set to 365 time steps (days).
- **Write model output files** – in calibration mode, the output files will contain the parameter sets of the most efficient parameter set for each SCE-UA evolution loop. You've already calibrated the soil zone, so you can switch this to 'N;'. You will need the parameter set information for the saturated and unsaturated zone though, so set these to 'Y'.

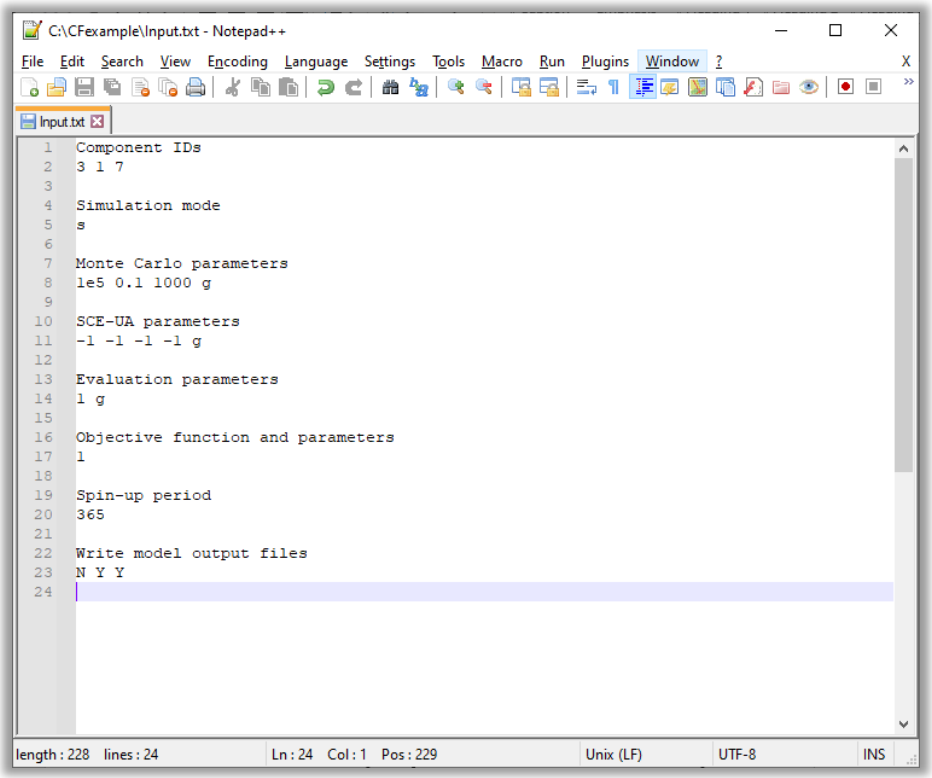

Figure 34: Configured Input.txt file for the Castle Farm SCE-UA calibration run.

6.5.3 Calibration input files

You calibrated the SMAP component in the previous tutorial, so **start by fixing all the parameters in the SMAP calibration input file (Calibration\SMAP_calib.txt) to those obtained from the SCE-UA calibration** (Output\SMAP_calib.out) (see Figure 35 for example). The Weibull and Q2K2S2 calibration input files have been pre-configured to suitable ranges based on the study site. In total, there are seven parameters to calibrate including the two Weibull parameters and five of the Q2K2S2 parameters.

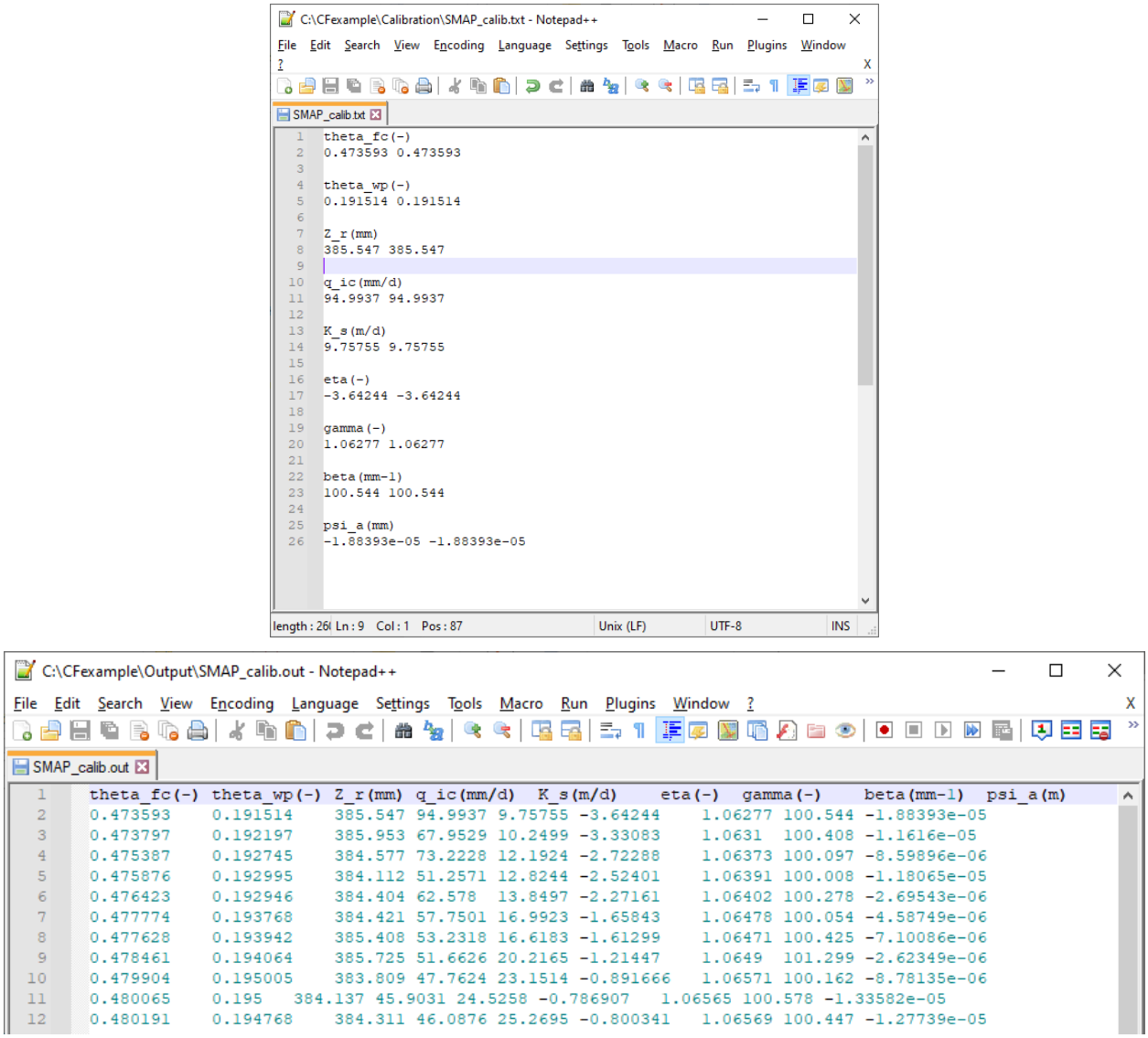

Figure 35: Calibration input file for the SMAP component (top) with parameters fixed based on the global optimum obtained from the SCE-UA calibration output file from the previous tutorial (bottom).

6.5.4 Running AquiMod 2 in SCE-UA calibration mode

Having configured the input files, AquiMod 2 is now ready to run. **Run AquiMod 2 in the command prompt**.

6.5.5 Output files

Navigate to the Output folder. AquiMod 2 should have produced a fit_calib.out, Weibull_calib.out and Q2K2S2_calib.out file. As in section 6.4.5 it is recommended that you experiment with modifying the SCE_n and SCE_p parameters to provide some reassurance that the SCE-UA approach has found a solution near the global optimum.

6.5.6 Model evaluation and comparison to other soil zone components.

Once that you are satisfied that you have obtained a solution in or around the global optimum, **configure AquiMod 2 to use this optimal model in evaluation mode** to obtain the groundwater level time series.

Repeat the SCE-UA calibration and evaluation for the other soil zone components (FAO and NSSS).

Figure 36 compares the calibrated models obtained using the three different soil zone components against the available groundwater level observation data. You can see that, in this case, all the models show very similar groundwater level dynamic behaviour and all of them broadly capture the observed groundwater level dynamics. This suggests that hydrogeological processes within the unsaturated and saturated zones are the dominant control on groundwater level variability given that the magnitude of soil drainage is known to be variable across the three models.

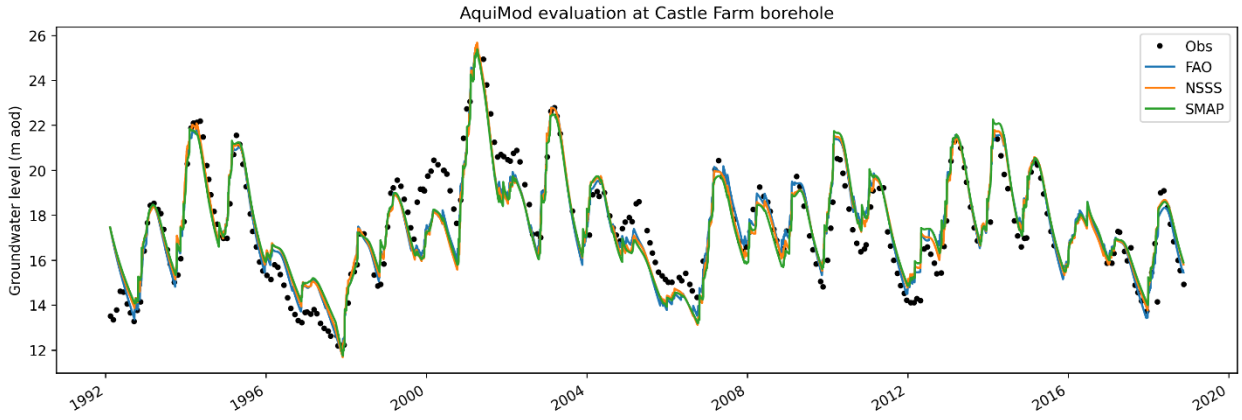

Figure 36: Simulated groundwater level time series against observations at Castle Farm observation borehole. Simulations are from the calibrated AquiMod 2 models using FAO, NSSS and SMAP soil zone components.

Appendix 1

List of output variables produced in time series files for each module component with variable file header, corresponding mathematical notation and description

SOIL ZONE COMPONENT OUTPUT VARIABLES

All soil zone component time series files have the same output variables

File header	Mathematical notation	Description (units)
q_ro(mm/d)	q_{ro}	Surface runoff (mm d^{-1})
E_a(mm/d)	E_a	Actual evapotranspiration rate from soil (mm d^{-1})
theta(-)	θ	Volumetric soil water content (-)
q_d(mm/d)	q_d	Soil drainage to unsaturated zone (mm d^{-1})

UNSATURATED ZONE COMPONENT OUTPUT VARIABLES

Weibull

File header	Mathematical notation	Description (units)
q_rech(mm/d)	q_{rech}	Recharge to the saturated zone (mm d^{-1})

SATURATED ZONE COMPONENT OUTPUT VARIABLES

Q3K3S1 and Q3K3S3

File header	Mathematical notation	Description (units)
Q_3(m3/d)	Q_3	Groundwater discharge from top aquifer layer (m^3 d^{-1})
Q_2(m3/d)	Q_2	Groundwater discharge from middle aquifer layer (m^3 d^{-1})
Q_1(m3/d)	Q_1	Groundwater discharge from bottom aquifer layer (m^3 d^{-1})
GWL(m)	h	Groundwater level (m above datum)

Q2K2S1 and Q2K2S2

File header	Mathematical notation	Description (units)
Q_2(m3/d)	Q_2	Groundwater discharge from top aquifer layer (m^3 d^{-1})
Q_1(m3/d)	Q_1	Groundwater discharge from bottom aquifer layer (m^3 d^{-1})
GWL(m)	h	Groundwater level (m above datum)

Q1K1S1, Q1T1S1 and VKD

File header	Mathematical notation	Description (units)
Q_1(m3/d)	Q_1	Groundwater discharge (m^3 d^{-1})
GWL(m)	h	Groundwater level (m above datum)

SA1D

File header	Mathematical notation	Description (units)
GWL(m)	h	Groundwater level (m above datum)

References

British Geological Survey holds most of the references listed below, and copies may be obtained via the library service subject to copyright legislation (contact libuser@bgs.ac.uk for details). The library catalogue is available at: https://of-ukrinerc.olib.oclc.org/folio/.

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