Future Flows and Groundwater Levels: R-Groundwater model summary

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Executive summary

This report is the result of research commissioned and funded by the Environment Agency's Science Programme, the Department for Environment, Food and Rural Affairs, UK Water Industry Research and the Natural Environment Research Council. It describes the structure of the R-Groundwater model that is used to simulate groundwater level hydrographs at a series of observation boreholes identified for analysis within the project.

R-Groundwater is a simple lumped catchment groundwater model written in the R programming language and run within the R environment. It has been developed to model groundwater level time series at observation boreholes by linking simple algorithms to simulate soil drainage, the transfer of water through the unsaturated zone and groundwater flow. Time-series of flow through the outlets of the groundwater store are also generated, which can be related to river flow measurements.

The model is calibrated through a Monte Carlo process by randomly selecting input parameter values from ranges specified by the user. Simple text files are used to define the input to the model and to write the output.

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Section I Structure of lumped catchment groundwater model

The R-Groundwater model consists of three components:

1. A soil moisture balance model producing a time-series of potential recharge (soil drainage).
2. A simple transfer function representing the delay in the time of the arrival of recharge from the base of the soil to the water table.
3. A lumped catchment groundwater model based on a simple Darcian representation of flow out of a series of aquifer “outlets”.

Each of these components is described in the following subsections. The structure of the model is shown in Figure 1.

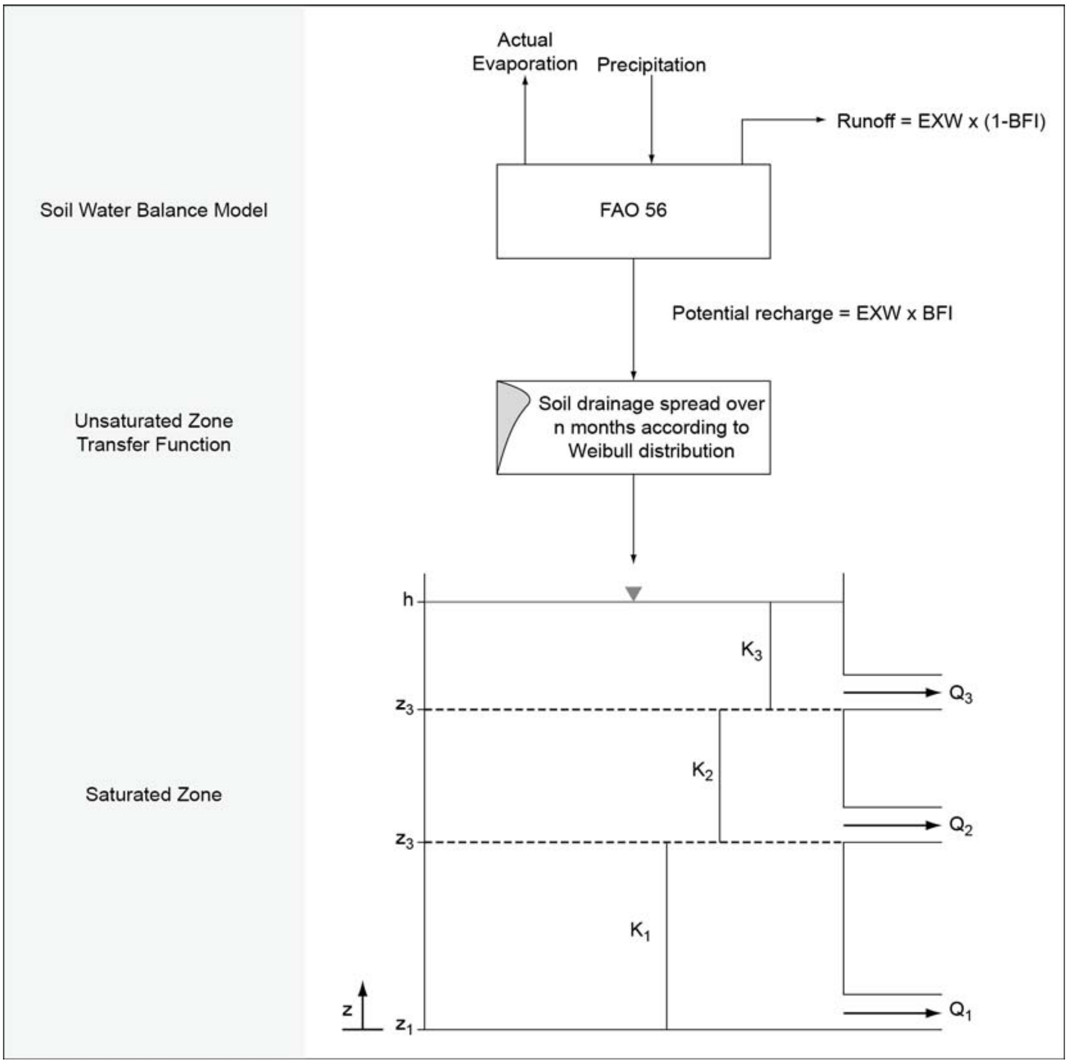

Figure 1 Structure of R-Groundwater model

I. 1 Soil moisture balance model

Potential recharge from the base of the soil zone is calculated using the FAO method (FAO, 1998), which describes soil moisture as a function of both vegetation root depth, and the propensity of vegetation to withdraw available water from the soil. Thus, this approach can appropriately represent soil moisture response to contrasting land-cover types.

In the FAO method, soil moisture is calculated using a maximum root depth (Z_r), and moisture depletion fraction (dp) parameter, which varies between vegetation and soil types. The amount of water available to plants after a soil has drained to its field capacity, is described as the total available water (TAW). TAW is defined as a function of the field capacity (FC), wilting point (WP) and maximum root depth (Z_r) such that:

$$TAW = Z_r \left(FC - WP\right) \qquad \text{Equation 1}$$

As the moisture content of the soil column decreases, vegetation will find it more difficult to extract moisture from the soil matrix. The fraction of TAW that can easily be extracted before this point, is reached is described as readily available water (RAW). The value of RAW is related to TAW by a land-cover defined depletion factor (dp):

$$RAW = dp\, TAW \qquad \text{Equation 2}$$

where Rf is the rainfall and SMD is the soil moisture deficit. The intermediate soil moisture deficit, SMD', is then:

$$SMD' = SMD_{(t-1)} + PE' - Rf \qquad \text{Equation 3}$$

where PE' is the potential evaporation. If in the above calculation SMD drops below RAW, the evaporation, AE, will take place at a lower rate determined by the equation:

$$AE = PE'\left[\frac{TAW - SMD`}{TAW - RAW}\right]^{0.2} \quad \text{when SMD` > RAW} \qquad \text{Equation 4a}$$

$$AE = PE' \quad \text{when SMD` ≤ RAW} \qquad \text{Equation 4b}$$

$$AE = 0 \quad \text{when SMD` ≥ TAW} \qquad \text{Equation 4c}$$

The calculation of SMD at the end of each timestep is then made with respect to the above, such that:

$$SMD(t) = SMD' + AE - PE' \qquad \text{Equation 5}$$

The excess water (EXW), or the amount of water that is available for surface runoff and potential groundwater recharge, is calculated as the amount of precipitation remaining after losses through interception, evapotranspiration, and soil moisture replenishment, such that:

$$EXW = Rf - AE - (SMD_{(t-1)} - SMD_{(t)}) \quad \text{when SMD ≥ 0} \qquad \text{Equation 6a}$$

$$EXW = SMD \quad \text{when SMD < 0} \qquad \text{Equation 6b}$$

The potential recharge, PR, is then calculated as:

$$PR = BFI \times EXW \qquad \text{Equation 7}$$

where BFI is the baseflow index. The parameters for FAO method can be based on those given in the FAO Irrigation and Drainage Paper 56 (FAO, 1998).

I. 2 Unsaturated zone transfer function

A commonly applied transfer function as used by Calver (1997) is the basis for the transfer of potential recharge from the base of the soil zone through the unsaturated zone to the water table. Potential recharge from the base of the soil in each month is applied to the water table over the current month and a number of subsequent months. The total number of months, n, over which recharge is distributed is a model parameter.

The distribution of recharge over the n months is specified using a two-parameter Weibull probability density function:

$$f(x;\lambda,k) = \begin{cases} \dfrac{\frac{k}{\lambda}\left(\frac{x}{\lambda}\right)^{k-1} e^{-(x/\lambda)^k}}{0} & x \geq 0, \\ & x < 0, \end{cases}$$ Equation 8

where k > 0 is the shape parameter and λ >0 is the scale parameter of the distribution. The resulting distribution is scaled such that the area under the curve is equal to unity and consequently the recharge for each time-step is simply spread over the selected, n, number of months. This Weibull function can represent exponentially increasing, exponentially decreasing, and positively and negatively skewed distributions as illustrated in Figure 2. It is used because it is smooth and considered to be more physically justifiable than randomly selected monthly weights.

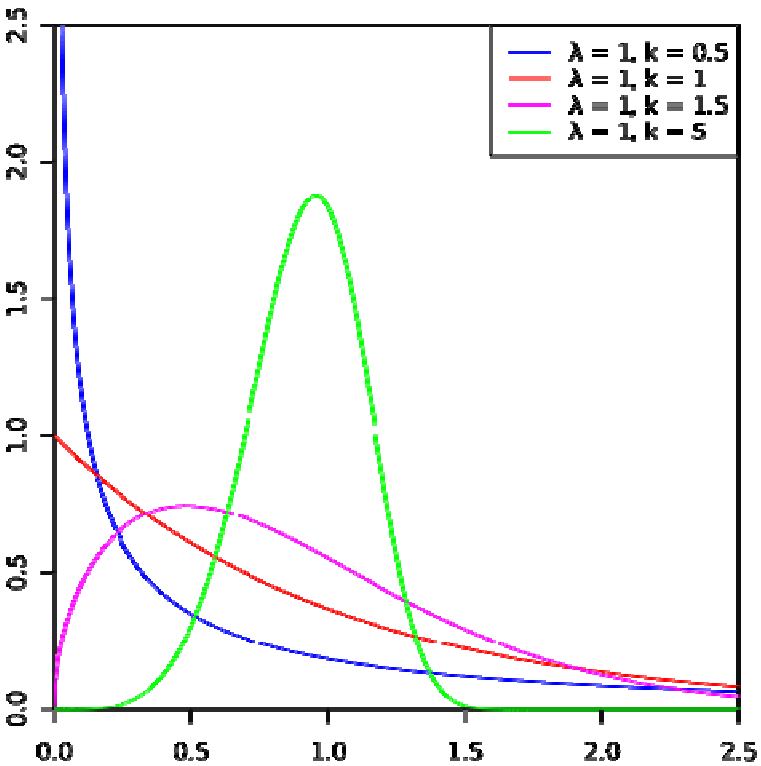

Figure 2 Example Weibull probability density function

I. 3 Lumped catchment groundwater model

Flow of saturated groundwater is represented by a rectangular block of aquifer. In the following description the aquifer is assumed to be unconfined but different aquifer conceptualisations can easily be accommodated. A simple, explicit mass balance calculation is performed at each time-step to calculate the new groundwater head. With reference to Figure 3 this mass balance is formulated as:

$$R\,\Delta x\,\Delta y - Q = S\,\Delta x\,\Delta y \cdot \delta h / \delta t \qquad \text{Equation 9}$$

where R is recharge [LT^{-1}], Δx and Δy are the length and width of the aquifer [L], Q is the groundwater discharge [L^3T^{-1}], S is the storage coefficient [-], δh is the change in groundwater head [L] over time, δt [T] and h is the groundwater head [L]. The discharge term, Q, is calculated using an equation of the form:

$$Q = \frac{T\,\Delta y}{0.5\Delta x}\Delta h \qquad \text{Equation 10}$$

where Δh [L] is the difference between the groundwater head and the elevation of an aquifer outlet point and T is the appropriately calculated transmissivity [L^2T^{-1}].

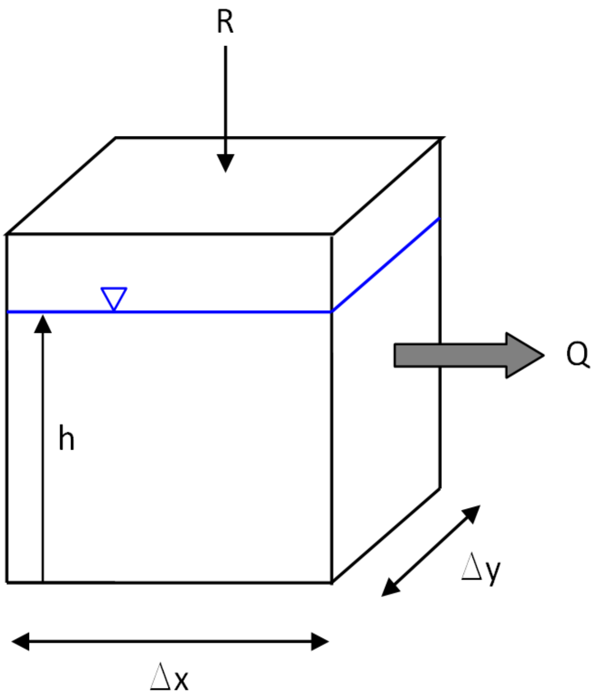

Figure 3 Basic structure of saturated groundwater model component

Groundwater flow out of the aquifer is split into a series of discharges via outlets at different elevations. Each of these outlets is associated with a vertical section of aquifer to which a value of hydraulic conductivity is specified (Figure 4). The aquifer is drained by a stream with perennial (Q_2) and intermittent (Q_3) flow components. A third discharge component (Q_1) is added at the base of the system to represent groundwater discharge below the level of a perennial stream. The groundwater level may fall beneath the level of the perennial stream (h_2) but will always be above the base of the aquifer (Z_1).

Hydraulic conductivity is defined using three piecewise constant values. The section of the aquifer discharging to the intermittent stream (above z_3) is characterised by hydraulic conductivity, K_3. The perennial stream is fed by a zone with hydraulic conductivity, K_2; and the groundwater discharge zone (below h_2) is controlled by a hydraulic conductivity, K_1. The storativity of the aquifer is depth invariant.

The discharge terms, Q, are again calculated using Equation 3 where Δh [L] is the difference between the groundwater head and the elevation of the outlet below, or the difference in elevation between two outlets, depending on the current groundwater head, and T is the appropriately calculated transmissivity [L^2T^{-1}].

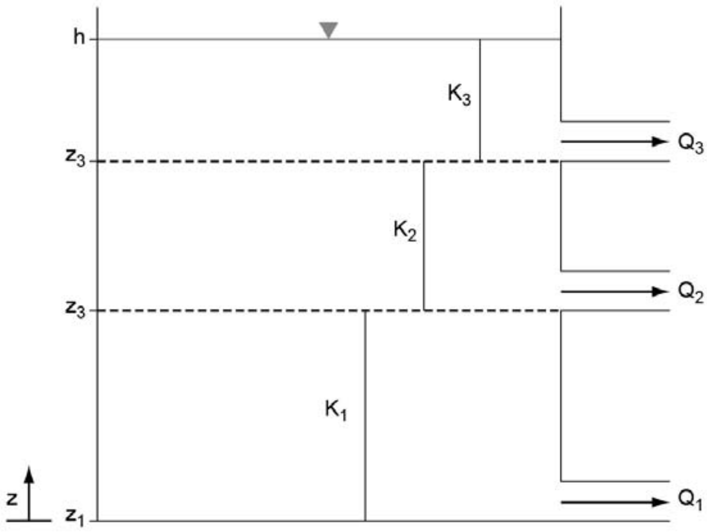

Figure 4 Saturated groundwater model component parameters

Section II Application of the model

The model is written in the R programming language. Individual models of groundwater level hydrographs are calibrated through a Monte Carlo process in which parameter values are sampled from user defined ranges. All of the model parameters can be defined as calibration parameters, however, some can be identified reasonably accurately based on hydrogeological judgment and are therefore fixed. A summary of the parameters for the model shown in Figure 4, and the data used to determine Monte Carlo calibration ranges for them, are listed in Table 1.

An example comparison between an observed and simulated chalk hydrograph using this model is shown in Figure 5.

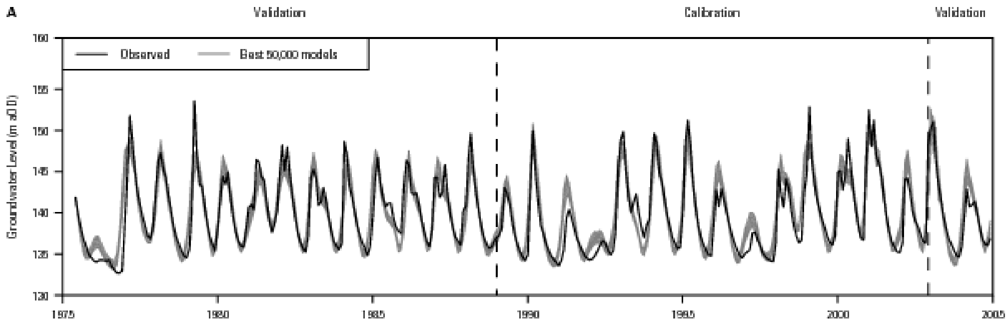

Figure 5 Observed and simulated hydrograph for the Baydon Hole borehole, Berkshire Downs.

II. 1 Input files

The model requires five input text files containing:

1. Model control parameters.
2. A times series of observed groundwater levels against which the model is calibrated.
3. Time-series of rainfall and potential evaporation.
4. An R file in which parameter value ranges for the soil moisture balance model and recharge transfer function are specified.
5. An R file in which parameter value ranges for the saturated groundwater model component are specified.

The format of these files is presented in Table 2 to Table 6.

Table 1 Summary of model parameters

Model component	Parameter	Data informing parameter estimation
Soil moisture balance	Runoff coefficient, RO	River base flow indices (1-BFI).
	Field capacity, FC	FAO Irrigation and Drainage paper 56 (FAO 1998).
	Wilting point , WP	FAO Irrigation and Drainage paper 56 (FAO 1998).
	Maximum rooting depth, Z_r	FAO Irrigation and Drainage paper 56 (FAO 1998).
	Depletion factor, dp	FAO Irrigation and Drainage paper 56 (FAO 1998).
Unsaturated zone transfer	Number of months over which to distribute potential recharge, n	Cross-correlation of monthly groundwater levels and lagged monthly rainfall.
	Weibull shape parameter, k	Calibration parameter but varied between values that allows a broad range of distributions to be tested.
	Weibull shape parameter, λ	Calibration parameter but varied between values that allows a broad range of distributions to be tested.
Saturated zone	Elevation of intermittent stream outlet, z_3	DTM elevation of intermittent streams.
	Elevation of Perennial stream outlet, z_2	DTM elevation of perennial streams.
	Elevation of groundwater discharge outlet, z_1	Geological and hydrogeological boreholes logs.
	Hydraulic conductivity, of upper aquifer (above z_3), K_3	Calibration ranges based on pump test data and hydrogeological experience.
	Hydraulic conductivity, of middle aquifer (between z_3 and z_2), K_2	Calibration ranges based on pump test data and hydrogeological experience.
	Hydraulic conductivity, of lower aquifer (between z_2 and z_1), K_1	Calibration ranges based on pump test data and hydrogeological experience.
	Storativity of aquifer, S	Calibration ranges based on pump test data and hydrogeological experience.

Table 2 Format of main input file "Input.txt"

Line	File contents	Description
1	---- Using the output from a previous run? (Y or N)	Comment line
2	N	Flag to determine if running previously calibrated models
3	---- If Y, run all behavioural models (i.e. that met error criterion)? (Y or N)	Comment line
4	N	Flag to determine if should re-run all behavioural models
5	---- If N, specify the number of best models to be used?	Comment line
6	10	If re-running subset of behavioural models how many should be run?
7	---- Recharge parameter input R file name	Comment line
8	Recharge_Model_Parameters.txt	Name of recharge model parameter input file
9	---- Groundwater parameters input R file name?	Comment line
10	Groundwater_Model_Parameters.txt	Name of recharge model parameter input file
11	---- Simulation start end date (format DD-MM-YYYY)	Comment line
12	15/01/1970	Simulation start date in dd/mm/yyyy format
13	15/12/1989	Simulation end date in dd/mm/yyyy format
14	---- Initial groundwater level	Comment line
15	16.8175	Initial groundwater head (m)
16	---- Number of Monte Carlo calibration runs	Comment line
17	1000000	Number of simulations in Monte Carlo run
18	---- Rainfall and PE data file name	Comment line
19	Rainfall_PE.txt	Name of rainfall and PE input file
20	---- Groundwater level file name	Comment line
21	Groundwater_levels.txt	Name of input file containing observed groundwater levels

Line	File contents	Description
22	---- Input directory	Comment line
23	E:\RModel\	Input directory path
24	---- Output directory	Comment line
25	E:\RModel\Results\	Output directory path (must exist before model is run)
26	---- Run name	Comment line
27	Example	Name of run which forms start of output file names
28	---- Error measure flag: 1=RMSE, 2=COREL, 3=RMSE of extreme values, 4=NSE	Comment line
29	1	Flag specifying which error measure to use
30	---- Error measure value (only those meeting criterion are stored)	Comment line
31	1.7	Error measure limiting criterion value for identifying behavioural models

Table 3 Format of observed groundwater level input file

File contents	Description
dt gwl	Header containing string "dt gwl"
1970-01-15 16.82	Date in yyyy-mm-dd format and groundwater level
1970-02-15 20.88	
1970-03-15 22.40	A space separated file
1970-04-15 21.81	
1970-05-15 21.91	
1970-06-15 20.66	
1970-07-15 19.46	
1970-08-15 17.96	
1970-09-15 16.68	
1970-10-15 15.46	
1970-11-15 14.28	
1970-12-15 13.75	
1971-01-15 14.39	
1971-02-15 16.18	
1971-03-15 19.42	
etc	

Table 4 Format of rainfall and PE input file

File contents	Description
dt pptn pe	Header containing string "dt pptn pe"
1970-01-15 72.0 12.0	Date in yyyy-mm-dd format followed by rainfall (mm) and PE (mm)
1970-02-15 70.9 24.2	
1970-03-15 65.0 40.6	A space separated file
1970-04-15 43.3 56.2	
1970-05-15 90.8 82.8	
1970-06-15 10.4 85.6	
1970-07-15 14.0 92.8	
1970-08-15 96.9 77.2	
1970-09-15 52.3 61.4	
1970-10-15 22.5 44.1	
1970-11-15 46.0 26.4	
1970-12-15 124.0 12.4	
1971-01-15 47.6 11.0	
etc	

Table 5 Example R file in which recharge model parameter ranges are defined

```
# Name of rainfall file? Change the name inside the ""
df.Rain.File=read.table("Rainfall_PE.txt",header=T)

# DO NOT MODIFY THE FOLLOWING 3 LINES
dt.Date.In=as.POSIXct(df.Rain.File$dt)
nu.Recharge.In=df.Rain.File$pptn/1000
nu.PE.In=df.Rain.File$pe/1000


# Parameters for the UZ transfer funtion
# Are the number of weights random or specfied (S/R)? (keep the " ")
ch.Calver.Weights.Choice="R"

# If R (random) give the range of the number of months over which potential recharge is spread
nu.Calver.Range.U=c(12,12)

# If S (specified) then give the monthly weights
# Monthly weights for transfer function (u)
nu.U=c(0.2,0.4,0.3,0.1)


# Are the Weibull distribution k and lambda random or specfied (S/R)? (keep the " ")
ch.Calver.Weibull.param.Choice="S"

# Range for Weibull distribution shape parameter k
nu.Wk.Range=c(2,6)

# Range for Weibull distribution scale parameter lambda
nu.Wlambda.Range=c(1.8,3.0)

# Runoff coefficient value equals one minus the base flow index
nu.ROCoeff=c(0.01,0.3)

# Soil parameter values ranges
nu.FC=c(0.2904,0.2904)
nu.WP=c(0.1529,0.1529)
nu.Zr=c(0.5,1.3)
nu.dp=c(0.02,0.2)
nu.SMDStart=c(0.0,0.0)
nu.PEAEFrac=c(0.1,0.1)
```

Table 6 Example R file in which groundwater model parameter ranges are defined

```
#-----------------------------
# SET PARAMETER RANGES BY CHANGING VALUES WITHIN c( , )

# Length of aquifer
nu.Length=c(4408,4408)

# K3 - Hydraulic conductivity for heads > Z3
nu.K.High=c(30,50)

# K2 - Hydraulic conductivity for heads > Z2
nu.K.Low=c(30,45)

# K1 - Hydraulic conductivity for < Z1
nu.K.Base=c(0.02,0.2)

# S - Storage coefficient
nu.S.Low=c(0.01,0.03)

# Z1 - Base elevation of the aquifer
nu.H.Low=c(-46,-46)

# Z2 - Outlet elevation for perennial river
nu.H.Mid=c(4,8)

# Z3 - Outlet elevation for ephemeral river
nu.H.High =c(6,23.5)

#-----------------------------
# DO NOT ALTER DATA BELOW HERE
# Dummy variables
nu.T.Low=c(10,500)
nu.T.High=c(500,5000)
nu.S.High=c(0.003,0.003)
nu.H.Mid2=c(120,140)
```

References

CALVER A. 1997. Recharge Response Functions. Hydrology and Earth System Sciences 1: 47-53.

FAO, 1998. Crop evapotranspiration; guidelines for computing crop water requirements, FAO Irrigation and Drainage Paper 56, Rome, 301pp.