WATSON
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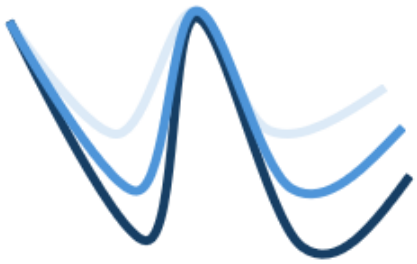
WITS- toolbox user manual:

Water
Isotope modeling for
Transit time and **S**torage



User manual to the WITS (Water Isotope modelling for Transit time and Storage) toolbox. Final report of working group 3 of COST Action CA19120: WATer isotopeS in the critical zONe from groundwater recharge to plant transpiration (WATSON)

https://watson-cost.eu/

Version 1.0

26.03.2025

This publication is based upon work from COST Action WATSON, CA19120, supported by COST (European Cooperation in Science and Technology).

User manual to the WITS software

DISCLAIMER

This report documents version 1.0 of the software WITS, a toolbox for estimating water transit times and storage volumes in the hydrological cycle. The toolbox is a collection of publicly available model codes. The different model codes implemented in this toolbox have been verified against a number of test cases. However, no warranty is given that the toolbox is completely error-free. If you do encounter problems with the code, find errors, or have suggestions for improvement, please contact info-wits@uu.nl.

The latest version of WITS can be downloaded from Github (https://github.com/srlutz/wits) and from the WATSON website (https://watson-cost.eu/storage-and-transit-time-estimation-in-hydrological-systems/).

The use of WITS can be acknowledged as follows:

Correa, A., Farlin, J. Lutz, S., Müller, S., Stockinger, M., The WITS-toolbox: Water Isotope modeling for Transit time and Storage. User manual, WITS, Version 1.0, Florence University, 27 pp., 2024.

Before you start

Please download the R programming language (https://cran.rstudio.com/). We recommend using Rstudio which can be downloaded here: https://posit.co/download/rstudio-desktop/). Also download the most recent version of the WITS toolbox from Github (https://github.com/srlutz/wits) or the WATSON website (https://watson-cost.eu/storage-and-transit-time-estimation-in-hydrological-systems/).

WITS can be used in any operating system supporting R. The developer team recommends using RStudio to avoid graphical issues with the predefined plots.

Contents

General Information

The WITS software implements different equations allowing the user to model tracer input-ouput problems related to hydrological systems. It is primarily intended to estimate the parameters of the transfer functions relating tracer input and output using the environmental isotopes tritium, deuterium and oxygen-18. Other tracers can be used with the software, bearing in mind that the concentration units might differ from those used for tritium (tritium unit, TU) and the two stable isotopes (per mille relative to a standard). The R code consists of a main driver file (**main_script_x_y.R** with "x_y" standing for the version of WITS) and several modules, each performing a given task (loading the data, pre-processing, parameter estimation and creation of the graphs). Users have two options to operate the software:

- Automatic Mode: Execute the entire R script as described in the quick guide and in the pages 14 to 18 of this report to navigate through different modeling options.
- Manual Mode: Experienced users can edit text files with a text editor and run modules sequentially. This approach requires R programming knowledge but offers more flexibility.

Code structure

This section presents the logical structure of the R code and the order, purpose and connections of the modules. All modules are called and executed from the driver file called **main_script_x_y.R** with "x_y" standing for the version of WITS. Each object's meaning within the modules is briefly explained after the "#" sign.

Calibration Process

The WITS calibration process occurs in multiple **runs**. Each run allows the user to change one modelling option without revisiting all other choices. Up to 20 runs can be performed. After each run, users decide whether to conduct another run. Before answering, the results of the run can be consulted and compared to previous runs. Results including graphical outputs, output tables, and parameter

run summaries are saved in folders named "run1" through "runxx" being the number of the last run.

Workspace definition and setup

In the first section of the main script, the user must edit the path to the folder containing the main script using a text editor and save the R file. By default, WITS utilized popup windows to guide users through all modelling choices. To disable these popup windows and input all choices manually in the corresponding module files (**user_choices_common.R**, **user_choices_LPM.R** and **user_choices_SAS.R**), the switch called **manual_input** has to be set to "1" instead of the default values of "0". If this is done, all user choices will be read automatically from the files **user_choices_common.R**, **user_choices_LPM.R** and **user_choices_SAS.R**.

packages_installation.R

This module loads all R libraries necessary to run the code. It checks if each library is installed on the computer, and if not, downloads it from an online repository, and loads it into the R session.

user_choices_xxx.R

All modelling choices are gathered in the three modules **user_choices_common.R**, **user_choices_LPM.R,** and **user_choices_SAS.R**. Choices appear one after the other via popup windows (default mode) or must be manually entered if popups are disabled (see "Section "workspace definition and setup""), entering the desired values, and saving the R files **before running WITS**.

Each of the modules is split into two sections:

- Automated Section: **if(manual_input=="N"),** it calls popup windows for choices.
- Manual Section: **if(manual_input=="Y")**, edit manually and SAVE BEFORE RUNNING THE CODE. Format and options for each object are indicated following the "#" sign.

The **time steps** for input and output can be user-defined. WITS requires regular time steps for the input. If the option "raw values" is chosen, the user must make sure that the input values are evenly spaced in time (for instance monthly values on the 15th of each month) and without gaps. All other choices for the input activate an algorithm that calculates mean values over each defined time step and then fill in the gaps (see section on input interpolation below). Output values may vary in spacing and resolution compared to input, permitting lower resolution calibration (for instance, monthly input values and annual output). Even if the option "raw values" is selected, the user is asked for the time step of the input. The

user defined value for "raw values" is equal to the number of time steps in a year (for instance 365 for daily data or 27.5 for bi-monthly measurements). This information is used to scale the calibration parameters that have units of time such as the mean transit time. Also, if tritium is used for modelling, the tritium decay half-life is scaled by the chosen time scale from its annual value. No warning will be issued if the value entered is erroneous.

Note

The object **offset_range** defined in **user_choices_LPM.R** and **user_choices_SAS.R** consists of an interval that is discretized by the number of steps given by **discretization** (user choice defined in **user_choices_common.R**). It is then used to scale up or down the predicted output to match the input by substracting from the predicted output all values between the minimum and the maximum offset and keeping the best fit.

The default interval (-5 to 5 TU/‰ for tritium/deuterium, -1 to 1 ‰ for oxygen-18) might in some cases be too narrow to increase or decrease sufficiently the mean value of the predicted output if the difference between mean input and output for the calibration period is greater than 5 TU/‰ or 1‰ for tritium, deuterium or oxygen-18 respectively. In such cases, the calibration algorithm usually selects the output that is the closest to a constant value as this minimizes the overall error, yielding a poor fit. To solve this potential issue:

- User Intervention: the user can either modify the input or the output or enter manually in the **user_choices_LPM.R** or **user_choices_SAS.R** an interval that better covers the systematic shift between input and output values.
- Explanation of Systematic Shifts: It remains the responsibility of the experimenter to explain such a systematic shift. For instance, differences due an altitude effect between the stations were the input and the output must be accounted for, or correct the input or the output accordingly.

Calibration can be performed using either a **single tracer** (tritium OR a stable isotope) or **both tracers** at once (i.e. the algorithm searches for a single parameter combination for the chosen model that explains both the tritium AND the stable isotope output for their respective input). When modelling a new dataset for which both tracers are available, it is **strongly advised** to start first by calibrating tritium and the stable isotope separately, both to make sure that WITS works as expected and to verify that good fits can be achieved with each isotope.

The **discretization** of the **parameter space** has a direct impact on calibration. A finer discretization improves the exploration of the a priori parameter space but increases dramatically calculation time. It is advised to begin with the suggested value of 10 steps and increase the number of steps only after WITS has been

successfully run to search for a better fit within the same parameter space or a subspace thereof.

input_interpolation_versionx_y.R

Unless the user has decided to work with the raw input values, the input time series is prepared at the time step chosen by the user (weekly, monthly or yearly) by calculating the average of all measurements within each time interval. Gaps (i.e. time steps without any measurements) are then interpolated linearly between the last value before the gap and the first value after it. Note that the average within each time step is **not weighted** by rainfall amount. If such a weighting is desired, the option "raw values" must be selected for the input and the weighting of the input data file prepared outside of WITS.

infiltration_coefficient_versionx_y.R

This module implements the equation proposed by Grabczak et al. (1984) to model evapotranspiration losses of environmental tracers by weighting the isotopic input of the summer months by a factor between 0 and 1. This factor is found from the difference between the average isotopic content in precipitation and at the outlet of the system of either oxygen-18 or deuterium:

$$\alpha = \left[\left(\overline{\delta P_w} - \delta G\right)\sum_i (P_i)_w\right] / \left[\left(\delta G - \overline{\delta P_s}\right)\sum_i (P_i)_s\right] \qquad \textit{eq. 1}$$

Where $\overline{\delta P}$ is the long-term mean weighted isotopic content in precipitation, δG is the mean isotopic content at the outlet, P is the precipitation amount, and s and w stand for summer and winter months respectively.The α factor is usually used to weight the tritium input (Grabczak, Małoszewski, Rozanski, & Zuber, 1984), whereby the measured values of the summer months are multiplied by α and if known, by the relative rainfall amount.

The α factor can also be applied to stable isotope input data when the average value in stable isotope output differs from the average value in input, under the reasoning that this difference is due to tracer losses by evapotranspiration during the summer months. The input is then (Maloszewski et al. 1992):

$$C_{\text{in}} = \frac{[N\alpha_{\text{i}} P_{\text{i}}(C_{\text{i}} - C_{\text{ground}})]}{\sum_{i=1}^{N}(\alpha_{\text{i}}\, P_{\text{i}})} + C_{\text{ground}} \qquad \textit{eq. 2}$$

With i =month number, α_i=1 for winter months and as defined in equation eq. 1 for the summer months and $\overline{C_{out}}$= mean isotopic value of the output.

Note

In moderate climates the alpha factor has a physical meaning if it is between 0 and 1 (0: no isotope contribution from the summer months, 1: no tracer losses through evapotranspiration during the summer months (Grabczak et al. (1984)). If however the average output is closer to the average input of the summer months rather than the winter months, the calculated alpha factor will be greater than one. Such a difference can be explained for instance by an altitude effect when the input sampling station is situated below the mean altitude of actual input. In that case, the WITS algorithm will calculate an alpha value greater than one and proceed with the weighting of the input summer months by increasing their value in a way that is not physical (i.e. by artificially creating mass in the case of tritium). No warning will be given by WITS.

monthly_average_versionx_y.R

This module calculates monthly averages for the tracer **output** if the option has been selected by the user. In case of variable flow, discharge is summed to create monthly sums.

annual_average_versionx_y.R

This module calculates yearly averages for the tracer **output** if the option has been selected by the user. In the case of variable flow, discharge is totaled up to create annual sums.

MTT_functions_versionx_yc.R

This module loads the different transfer functions implemented in WITS. Experienced users can program new functions here if desired.

MTT_functions_versionx_yd.R

This module replaces the existing transfer functions with their variable flow equivalents if the variable flow option has been selected. This is where the experienced user can program new functions if desired.

Note

Not all transfer functions available for the steady-state formulation are available for variable flow calculations.

calibration_data.R

This module prepares all the input and output data used for calibration depending on the selected options. This includes the choice of one or two tracers,

a complete output time series or subset used for calibration, and additional variables if variable flow is to be simulated.

calibration_setup.R

This module prepares all the output directories where the calibration results and the graphical outputs are stored.

monte_carlo_setup.R

This module prepares all the vectors for the parameters that will be varied during calibration. Each vector contains the minimum and maximum value of the corresponding parameter.

monte_carlo_LPM.R and monte_carlo_SAS.R

These two modules calculate and save the computed output vector for all parameter combinations as well as the corresponding measure of fit. Depending on the user choice (classical lumped parameter models or storage selection functions), either **monte_carlo_LPM.R** or **monte_carlo_SAS.R** will be activated for the convolution. WITS uses a brute force algorithm that calculates all parameter combinations instead of trying to improve fit iteratively. The best fit is then searched in the next module (**parameter_estimation_LPM.R** and **parameter_estimation_SAS.R**). For each **fitting parameter**, a vector is defined with equal steps between the minimum and maximum values given by the user. How finely the parameter space will be explored depends on the parameter interval and on the chosen **discretization** (i.e. how many steps have been chosen. See **user_choices_xxx.R**). A finer discretization improves the precision of the search for the best fit but increases calculation time.

parameter_estimation_LPM.R and parameter_estimation_SAS.R

These two modules identify and save the best fit according to the selected measure of fit (Nash-Sutcliff or mean prediction error). They also prepare ensemble solutions with measures of fit better than a specified percentage threshold among all computed fits. The default value for the threshold is 5% (i.e. the 5% best solutions are retained). If multi-objective calibration is performed (two tracers at once), the best compromise solution is searched among the parameter combinations yielding measures of fit within the 5% best solutions for tritium AND the stable isotope. If no solution can be found in the subset, the threshold is increased incrementally by 0.5% until a common best fit is found (the compromise solution).

Note

Because the best compromise solution is searched within the best fits for tritium first, the absolute tritium best fit and the compromise solution for tritium will be the same. This however means that the compromise solution for the stable isotope will often yield a worst fit than the absolute best solution obtained by calibrating a model using the stable isotope only.

Depending on the user choice (classical lumped parameter models or storage selection functions), either **parameter_estimation_LPM.R** or **parameter_estimation_SAS.R** will be activated for the convolution.

parameter_run_summary_LPM.R and parameter_run_summary_SAS.R

These two modules prepare and save a CSV file containing all the input parameters of the run.

graphics_labels_boundaries.R

This module prepares labels for graphical outputs and calculates the boundaries for the x and y axes.

graphics_inputs.R

This module creates a graphical output for the input time series.

graphics_outputs.R

This module creates a graphical output for the output time series as well as the following graphs: (i) fitted transit time distributions, (ii) time series and (iii) boxplots of the residuals.

Trouble shooting

This section presents commonly encountered issues running WITS and their respective solution.

Complexity

When setting up a new model, the user is advised to start with the simplest possible setup in order to check that WITS runs within an acceptable computation timeswith the new input and output data and the chosen time steps. Once this has been verified, complexity and discretization of the parameter space can be increased to the level required by the question at hand.

Wrong date format

The only date format recognized by WITS is YYYY-MM-DD (for instance "2021-01-15" for the 15th of January 2021). Other date formats will not generate directly an error message but will cause the calibration algorithm to fail. Solution: Double check the date format to ensure compliance.

Output measurements extending beyond the input

WITS does not extrapolate the predicted output beyond the last input measurement available. Thus, if the input data vector finishes earlier in time than the output data vector, the calibration algorithm will fail. Solution: Verify that the last input value extends beyond the last output measurement.

NA and missing values in the raw data

WITS contains an algorithm to check and remove NA and missing values. It may however fail in some cases, depending on the denomination used ("NA", "NaN", "not measured", etc..), causing the convolution to fail. Solution: The user is advised to remove NA and missing values from the raw data files before loading them in WITS.

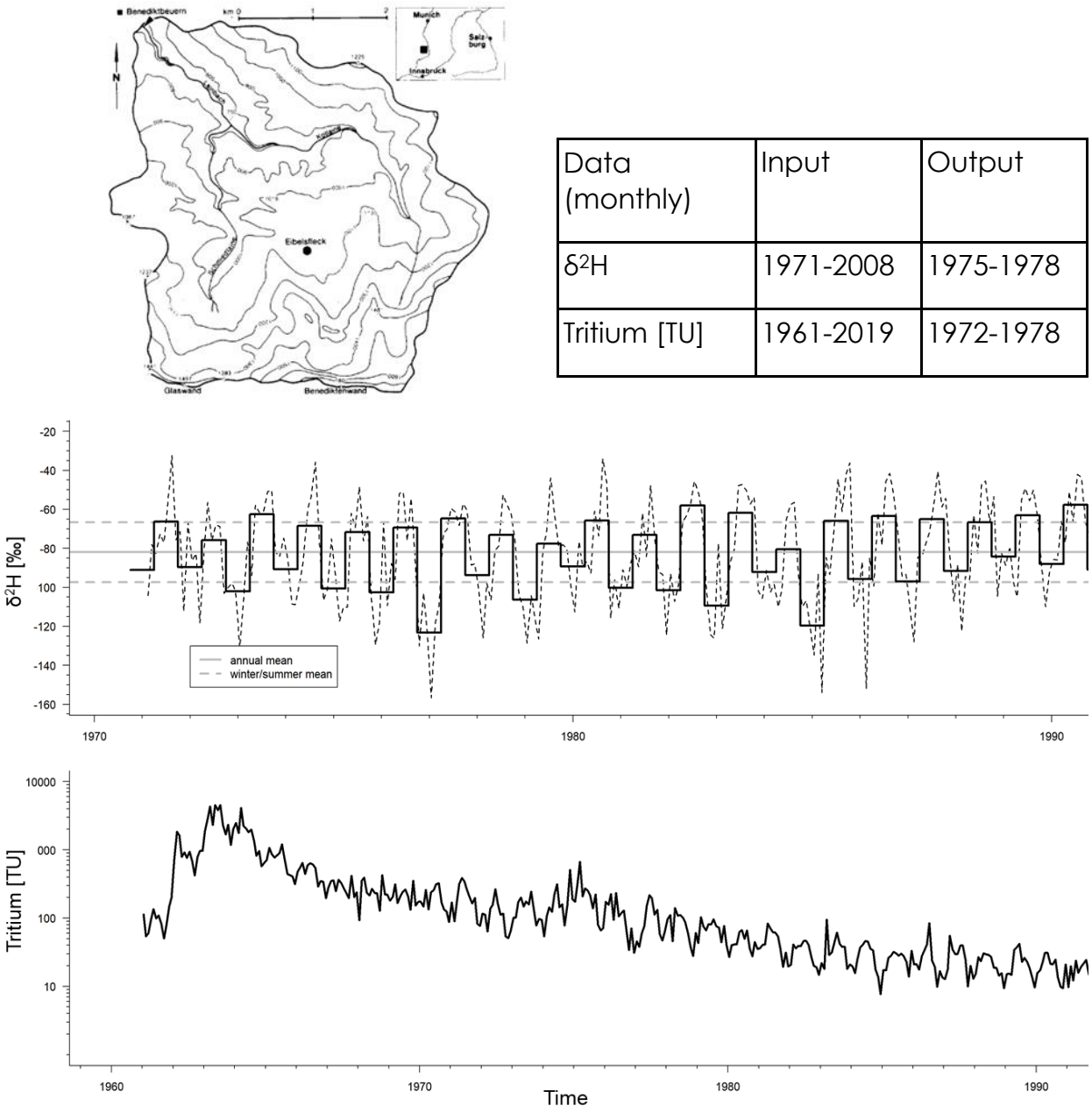
Running WITS

This section presents the use of WITS for a simple case study. In this example, the data is in the folder ´**\data\additional_data**´. The data folder used by WITS is ´**\data\raw**´, so the sample data is also already copied into that folder. The main executable script and necessary model functions can be found in ´**\src…**´. Additional literature and the User Guide can be found ´**\docs…**´. The results of successful model executions are stored in ´**\results…**´. The toolbox provides a basic graphical output for ad-hoc visual evaluation of the model results, but the users are encouraged to create their own graphical output once satisfied with the modelling results. The raw data of the simulated output is stored in ´.txt-file format´.

Input data

For this example, we use data from the Lainbach catchment (

Figure 1) to demonstrate how WITS operates with real-world datasets.



Data (monthly)	Input	Output
δ^2H	1971-2008	1975-1978
Tritium [TU]	1961-2019	1972-1978

Figure 1. Example of input data to the model. This quick guide uses data from the Lainbach catchment south of Munich, Germany (detailed map, top row left). Various isotope data is available for that station or the nearest tritium precipitation sampling station (Vienna). The center plot shows a 20-year deuterium (δ^2H) time series (dashed lines) and their respective six-month mean values for summer and winter periods. The lower plot shows the atmospheric tritium concentration reconstructed for the closest tritium measurement station in Vienna.

Running the script

First, browse to the respective folder, where you installed the toolbox. Go to ´**\src…**´ and load and execute the main script in RStudio: ´**main_script_1_0.R**´.

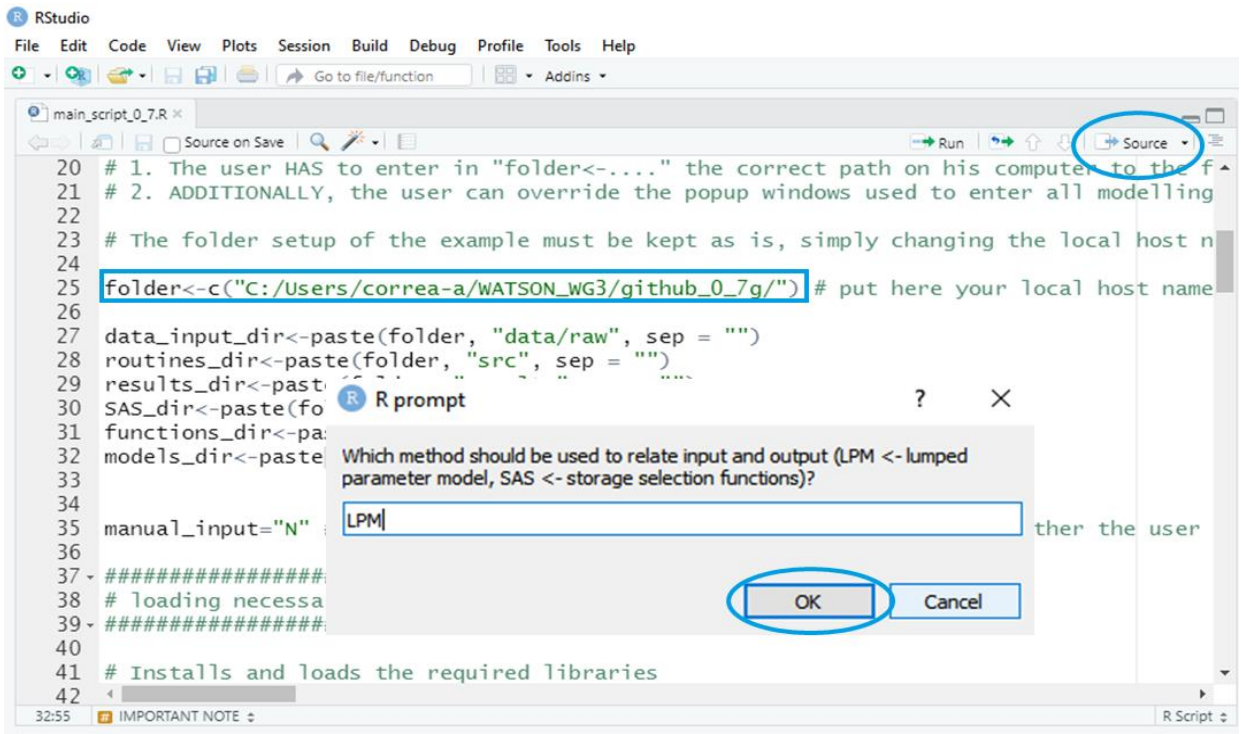
The folder setup of the example must be kept as is, simply changing the local host name to the main folder

folder<-c("C:/exampleuser/exampleuser/exampleWITS/exampleWITSversion/")

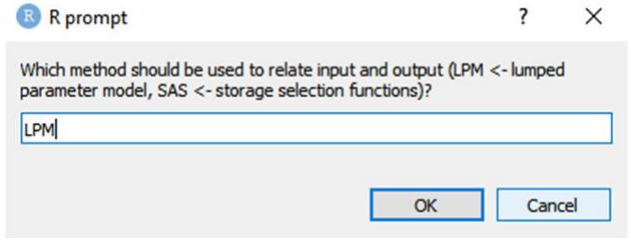
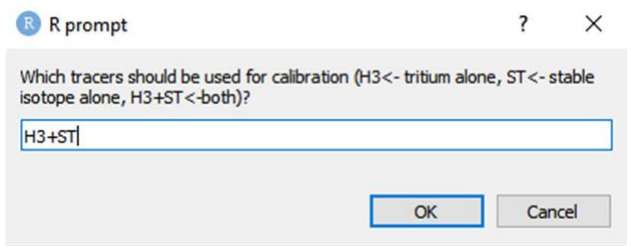
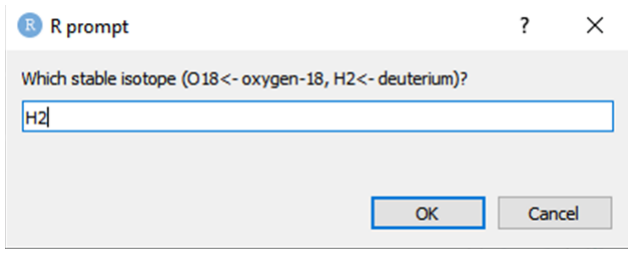
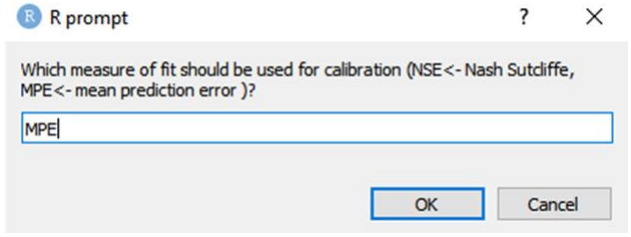
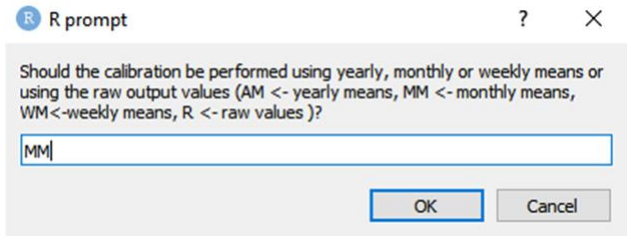
put here your local host name.

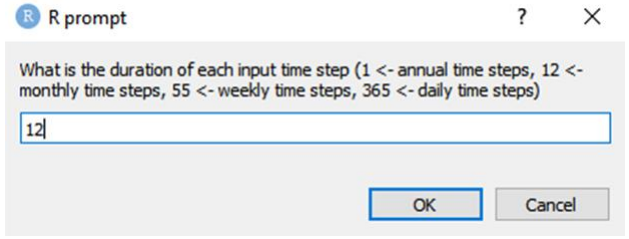
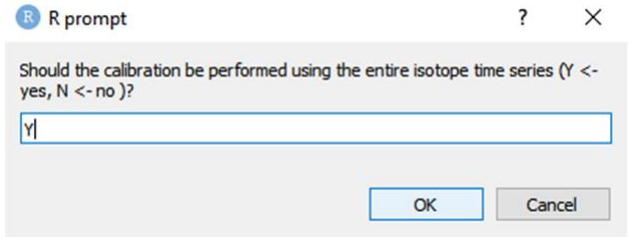
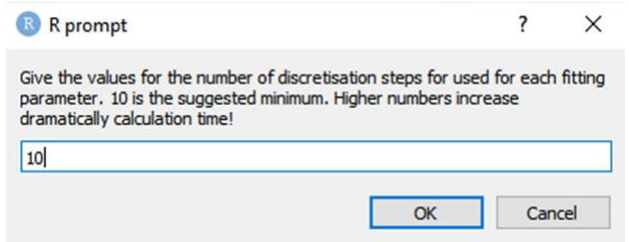
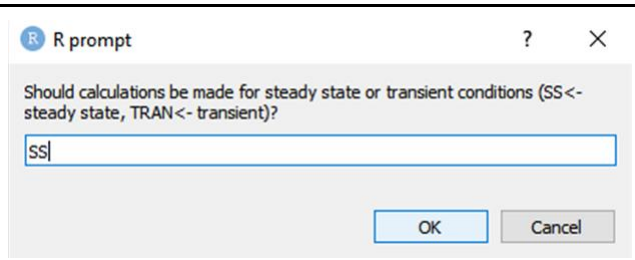
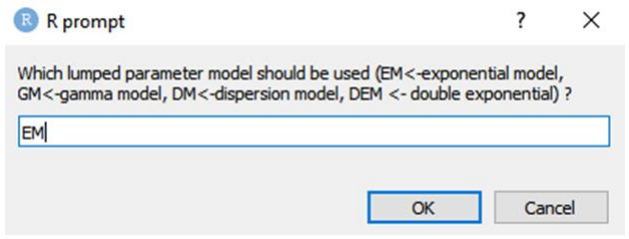
The options selected in this guide are the ones **used by the authors,** we recommend using the same settings for your initial run to familiarize yourself with WITS. This will help you to follow along with the guide and understand the process step by step.

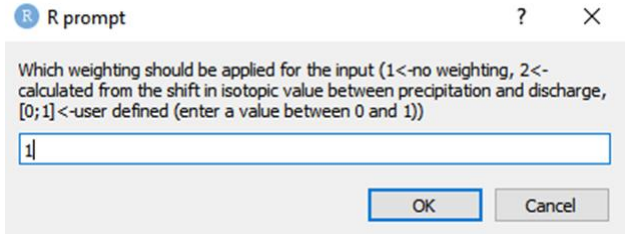
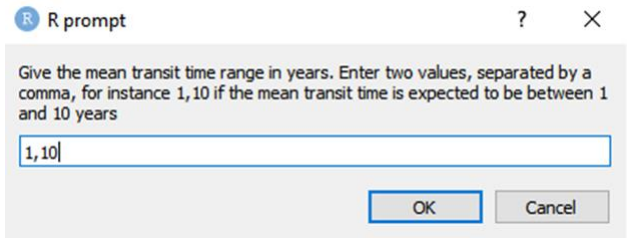
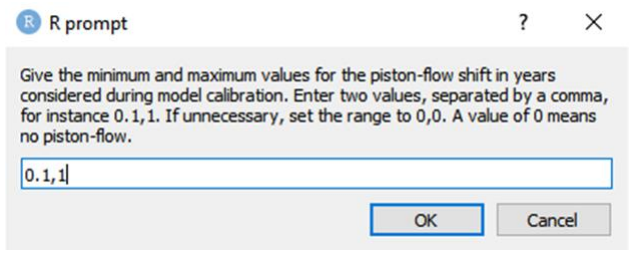
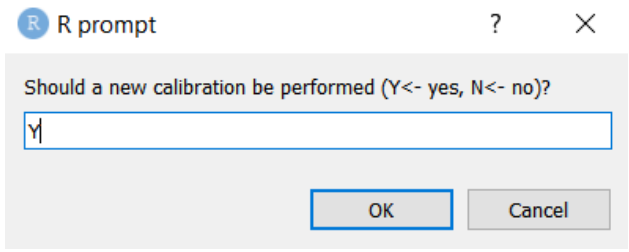
To run the script, click on "Source." Pop-up windows will appear, allowing you to customize your preferences for running the script. Once you've selected your options, click "OK" to proceed with the next steps (as shown in the graphic below).

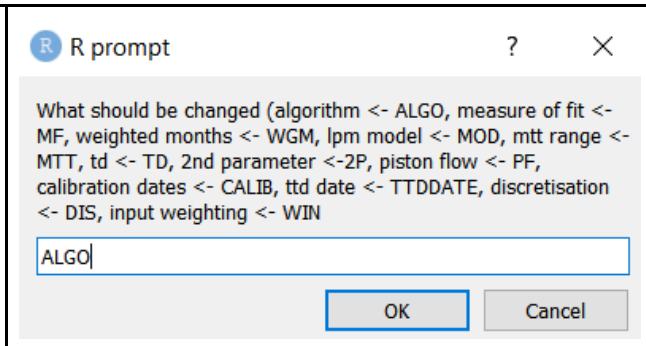


Please continue selecting your options in the following windows, adjust them according to your needs. Follow the prompts until the process is complete.

C.1		**Define the Model Type:** Choose between the Lumped Parameter Model (LPM) for Transit Time Distribution (TTD) curves and Mean Transit Time (MTT) estimates, or StorAgeSelection functions for storage volume and transit time age estimates.
C.2		**Select Tracers:** Two tracer types are available: Tritium (H3) and Stable Isotopes (ST). For this guide, Deuterium (H2) was selected. If both tracers are selected for calibration, the calibration is implemented in a stepwise manner. First, the parameters from the best 10% solutions based on tritium as calibration target are found and retained. Within this parameter subset, the best solution for stable isotopes is found.
C.3		**Please Select the stable isotope:** Oxigen-18 (O^{18})or deuterium (H^{2}).
C.4		**Calibration Metrics:** Choose a measure of fit for calibration. We recommend Mean Predictor Error (MPE) for quicker calculations. Nash-Sutcliffe Efficiency (NSE) requires longer processing time.
C.5		**Input Data Frequency**: The preprocessing script can calculate mean values based on different time intervals: Yearly (AM) Monthly (MM) Weekly (WM). If "raw values" is selected, data gaps in the input will not be filled in by interpolation and will cause an error message.

C.6		**Time Step Duration**: Specify the duration of the input concentration time steps to match the model requirements. Downscaling (i.e., from daily to hourly) of input data is not implemented and will not work. If selected time step is larger than input time step (i.e., minute data to daily), the data is aggregated to the desired time step (the mean is calculated). If the user requires another aggregation time step, it has to be done outside the WITS toolbox.
C.7		**Isotope Time Series for Calibration:** Decide whether to use the entire isotope time series of the catchment output concentration for calibration (Y/N). If "No," is selected the user is then asked to define the specific period for calibration themselves.
C.8		**Discretization Steps:** Select the number of discretization steps for each fitting parameter. A minimum of 10 steps is recommended for adequate discretization, however, it is important to note that 10 steps is rather coarse. Higher discretization of the parameter space will increase computational speed.
C.9		**Model Conditions**: Choose between Steady-State (SS) or Transient (TRAN) conditions based on your catchment's behavior. Here, steady state (no storage and flow rate change) was selected for the Lainbach catchment. If transient is selected, a variable flow and storage is calculated.
C.10		**Lumped Parameter Model:** Choose the model you wish to apply: Exponential Model (EM) Gamma Model (GM) Dispersion Model (DM) Double Exponential Model (DEM). For variable flow, only EM and DM will be offered.

C.11		**Data Weighting:** Select whether to apply weighting to the input data: 1 = No weighting 2 = Weighting based on the shift between input and output isotope time series Or, define a custom weighting value between 0 and 1. Note, if summer rainfall does not contribute to the overall isotope signal in the output signal, weighting may be necessary. Hence, if weighting is set to a number below "1" for specific month (user defined in a follow up pop-up window), the isotopic signal is reduced by that weighting factor, compared to the non-weighted month.
C.12		**Transit Time Range:** Define the estimated range expected for transit time, using a minimum and maximum value separated by a comma. Example: (1, 10). Within this transit time range the best solution is searched for.
C.13		**Piston-Flow Consideration:** If your system should include piston-flow, specify the shift (in years) for calibration by entering a minimum and maximum value separated by a comma. Use (0, 0) if piston-flow is not present.)
C.14		**After the first execution:** Confirm if you wish to perform another run by selecting Y or N. Choose Y to rerun the process, or N to exit.

C.15		**After selecting to rerun the process: You can** configure the following alternatives: • Algorithm • Measure of Fit • Weighted Months • Lumped Parameter Model type • Mean Transit Time Range Among others.

Results

The results will be presented in folders with the following structure (Figure 2. two tracers are used):

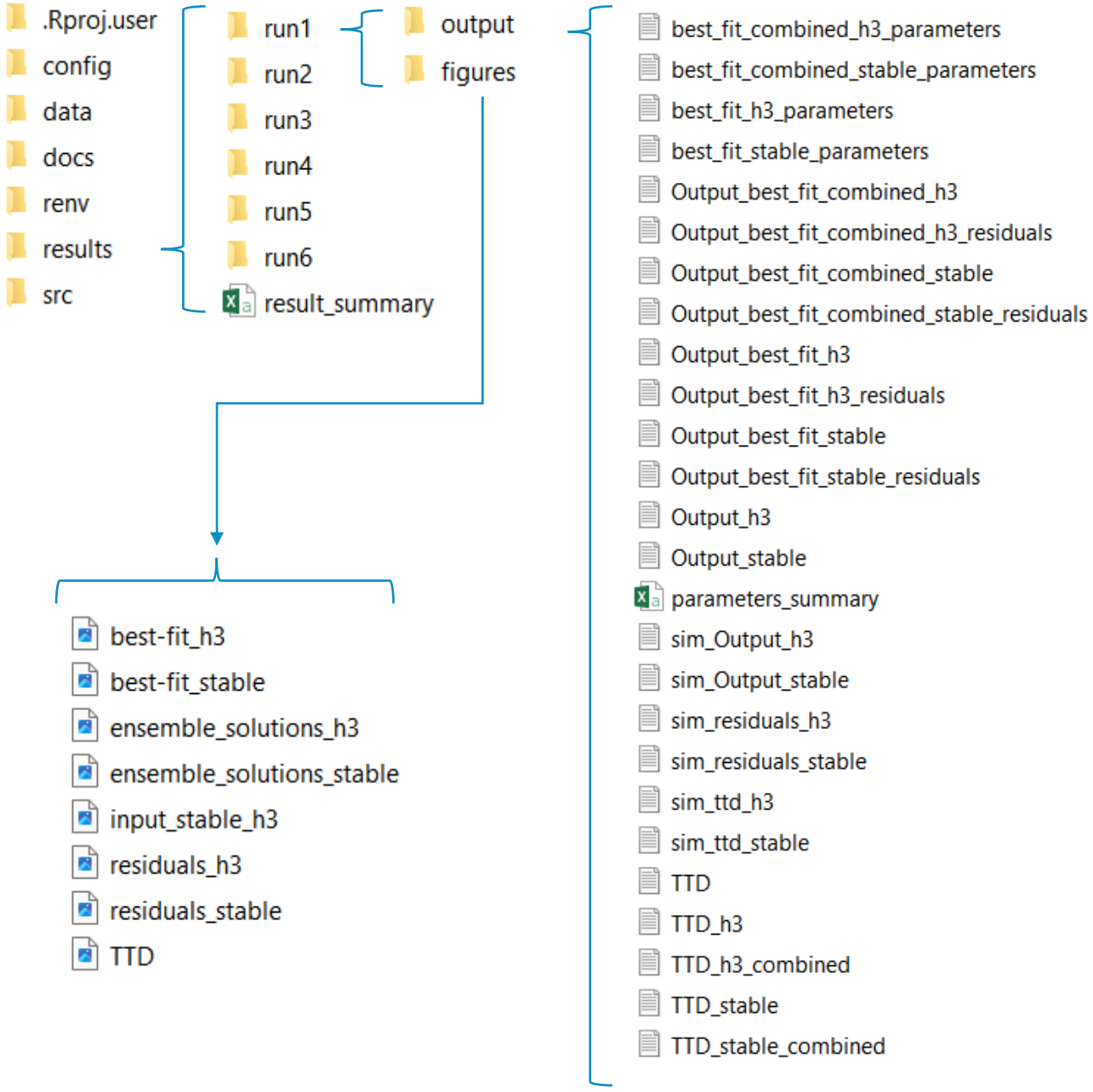


Figure 2. Structure of result folders and output files. Detailed description on each file type can be found in Table 2.

Results: Output Tables

If two tracers are used, a combined best fit table will be generated (Figure 2). This means that a combined table will summarize the best fit parameters for both tracers.

Each folder will contain multiple runs (e.g., Run 1 through Run 6 in the example). A total of up to 10 runs can be performed. In addition to the individual run folders, a summary text file will be generated, providing a summary of the results.

Inside each run folder, a series of text files are presented. These files include detailed outputs from the simulation, as well as a file with the summary of parameters (Table 1). The content of each specific files is described in Table 2.

Please note, that the "output" folder shows essentially **five categories** of files starting with **"best_fit_[…]", "Output best fit_[…]","output[…], "sim_[…]", "TTD_[…]"**.

For each category there are **three content groups**. The content in each groups is either the parameter table which is extended by **[…]_parameters**, or a timeseries of residuals extended by **[…]_residual**. The simulated best- fit isotope timeseries does **not** contain any **additional name** extension.

To those overall categories and content groups the name is finally extended depending on the chosen **isotope configuration** of the model. If only one isotope is chosen for calibration then names are either **"[…]_H3" (tritium)** or **"[…]_stable"** (deuterium or oxygen-18). If two isotopes are chosen then the name of the relative best fits output files is extended by that information such as **"[…]_combined".**

Table 1. Example of Parameter Summary for an Individual Run.

algorithm	fit	weight	Months	model	mtt	pf
BF	MPE	1	1	EM	2	0.1
BF	MPE	1	2	EM	5	1
BF	MPE	1	3	EM	2	0.1
BF	MPE	1	4	EM	5	1
BF	MPE	1	5	EM	2	0.1
BF	MPE	1	6	EM	5	1
BF	MPE	1	7	EM	2	0.1
BF	MPE	1	8	EM	5	1
BF	MPE	1	9	EM	2	0.1
BF	MPE	1	10	EM	5	1
BF	MPE	1	11	EM	2	0.1
BF	MPE	1	12	EM	5	1

Table 2. Description of the content of the text files contained in the folder "output"

Category	Content	Description
´best_fit´[…]	´best_fit_[...]_**parameters**´ ´best_fit_combined_[...]_**parameters**´	This section contains the **parameters** that yielded the best model fit. This can be either the best fit model output for each individual tracer (stable or tritium) or the combined output if two tracers are used.
´output_best_fit_[...]	´output_best_fit_stable ´ ´output_best_fit_H3 ´ ´output_best_fit_combined_stable_residuals´ ´output_best_fit_combined_H3_residuals´	This file contains the absolute best fit of the prediced **isotope concentration** per timestep for each individual tracer (stable or tritium), or if two tracers are used the relative best fit that minimizes the residuals of both tracers. If **residuals** are attached in the name, the file contains the residuals of the fit (i.e. observed versus predicted output for each observation date).
´output_[...]´	´output_H3 ´ ´output_stable ´	This file contains a list all parameter combinations and their respective error for all simulation runs.
´sim_[…]´	´sim_output_[...]´, ´sim_residuals_[...]´ ´sim_ttd_[...]´	Those files contains a **record of all simulation runs** and their respective predicted isotope value per timestep ([…]_output), **their residuals** per timestep ([…]_residuals) and the **g(t)** per timestep ([…]_ttd. Be aware this table is transposed so that the time is along rows (including header D[…] or X[…] in the first row) and columns show individual runs.
´TTD[...]´	´TTD´ ´ TTD _H3´ ´ TTD _stable´ ´ TTD _H3_combined´ ´ TTD _stable_combined´	This table gives the probability distribution **g(t)** for the **best fit** simulation. ´ TTD ´ is generated when only a single tracer is used. When two tracers are used, the 'TTD' is generated for each single isotope tracer. Note: Since in the case of the simultaneous fitting of two tracer the best 10 % solutions the all tritium simulations are retained before looking for the best stable isotope simulation amongst those, ´TTD_H3_combined´

		´TTD_stable_combined´ and will be the same as to ´TTD_H3´.
´parameter_summary´	-	Summarizes all input parameters used for this specific run.

Results: Output Figures

The output figures are stored in the *results folder (Figure 2). Each run is in a separate directory labelled "runxx". Each "run" directory contains two folders. The "figures" folder contains all the graphs showing the input and fitted output. The "output" folder contains the data tables generated.* The user finds scatter plots (XY plots) showing the best fit for stable isotopes and tritium individually, along with their residual errors presented as a time series and box plots displaying the distribution of the residuals. An example is shown in Figure 3.

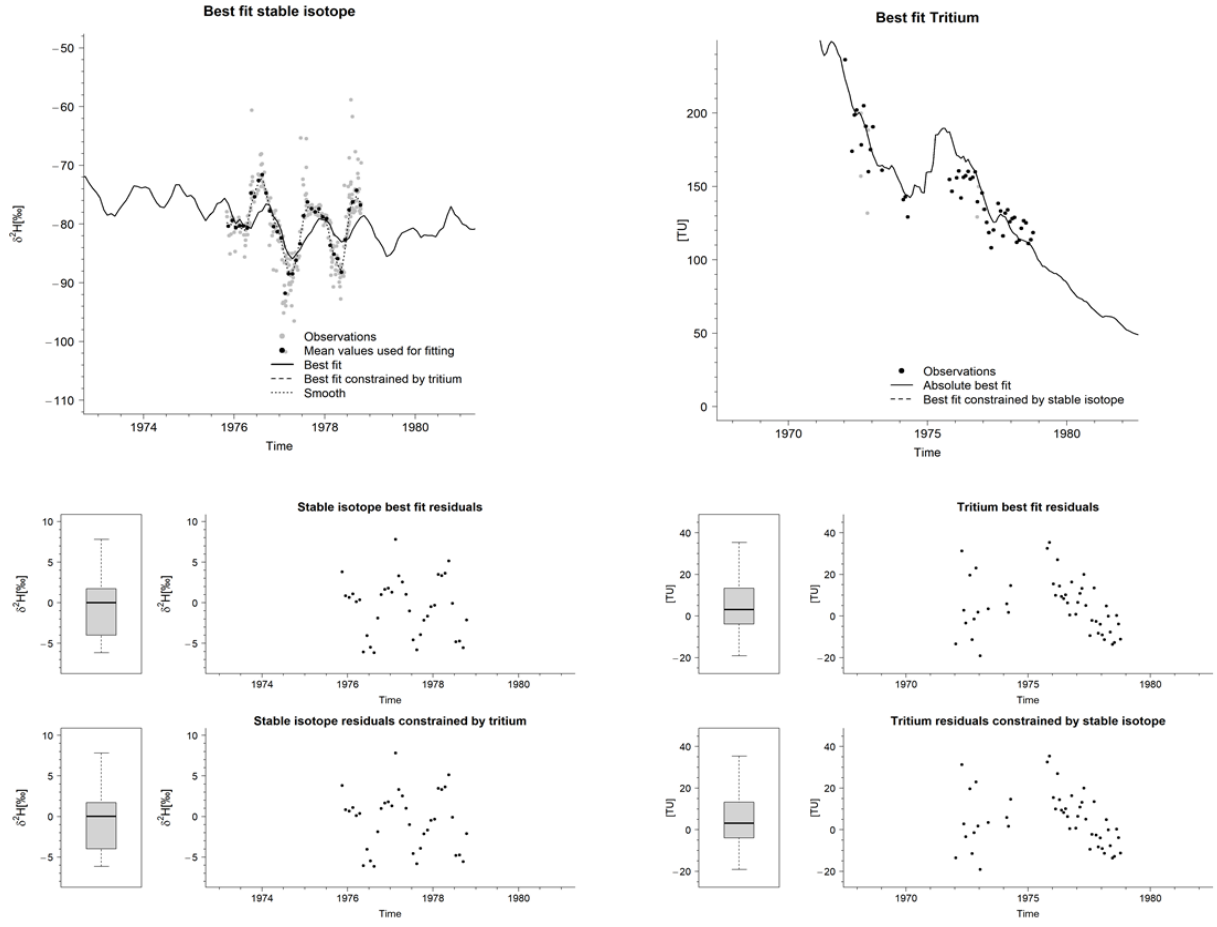


Figure 3. Various results figures produced automatically by the WITS toolbox. The header of each shows the content presented. Here the best-fit time series of the stable isotopes (upper left) and best fit tritium (upper right) is shown. If an analytical error is provided with the tritium data, it will be shown as error bars on the graph. The center row and bottom row presents residuals of the stable isotope tracer and tritium tracer,

respectively. The bottom figure will be produced if both a stable and a radioactive tracer is used for calibration. The raw data of those figures is stored in the corresponding subfolder "output". Users are encouraged to develop their own plots for potential publication.

Figure 4 shows the transit time distribution, as well as the ensemble solutions for tritium and the stable isotope. For the latter, it includes observed samples and the ensemble solutions, which represent the best 1% of all simulations, along with their respective best fit. This selection of ensemble solutions is defined based on performance criteria that identify the most accurate simulations in relation to the observed data.

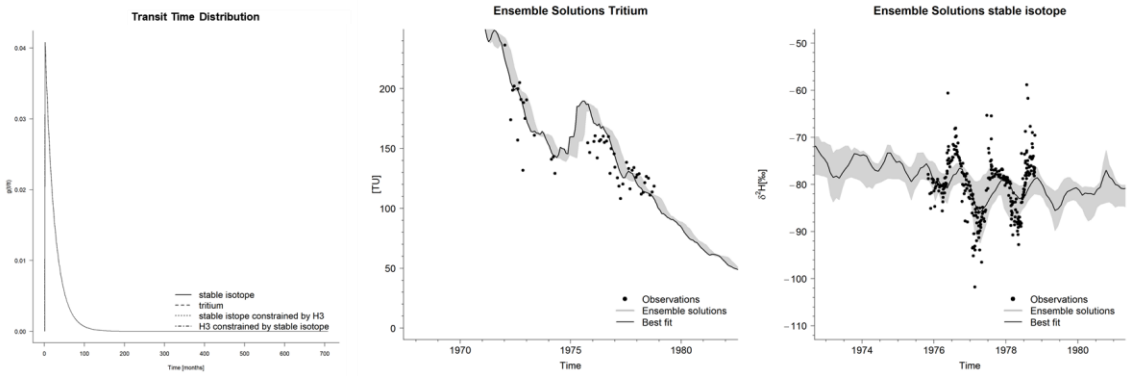


Figure 4. Other graphs stored in the "figure" folder. The left figure shows the transit time distribution of the best fit solution. The center and right plot shows an ensemble solution of tritium and stable isotope estimates. Ensemble solutions represent the best "1%" of all solutions.

Data requirements

For details on data requirements for each method please read the **´Final report of working group 3 of the COST ACTION WATSON´.** Before using your own data for modelling please familiarize yourself with the model implementations in order to ensure a correct interpretation of the model results.

The user has to ensure a continuous data series of similar time steps. Data gaps in the time series are automatically filled in by WITS with simple linear interpolation between two data points. This may introduce unwanted errors. We encourage the User to ensure that potential gap filling errors are corrected before modelling is conducted.

The model does produce false results with mixed input data time steps (e.g.: one year of daily data, and 5 years of monthly data). Aggregation outside the WITS software to the desired time step is strongly advised.

- The user has to provide at least one isotope time series of catchment input and output to meet minimum requirement for the LPM models.

- SAS models require a minimum of four input variables for variable flow calculations: precipitation, evapotranspiration, discharge and a single isotope time series of the input and output.

When using your own data, make sure to set it up using the criteria described in the table 3. Please use the exact file name for each file as written in the table 3. Decimal places are separated by "." (dots) while columns are separated by "," (comma) and the input file type is ".csv".

Table 3. Input files and format criteria. Decimal seperator is "." (dot) and column separator is "," (comma.

File type	**File name**	**File format and columns names**
LPM		
Stable isotope input timerseries	stable_input.csv	Date,isotope [YYYY-MM-DD],numeric value
Stable isotope output timerseries	stable_outpu.csvt	Date,isotope [YYYY-MM-DD],numeric value
Tritium input timeseries	h3_input.csv	Date,H3 [YYYY-MM-DD],numeric value
Tritium output timeseries	h3_outputt.csv	Date,H3 [YYYY-MM-DD],numeric value
LPM (transient)		
Discharge	discharge.csv	Date,J [YYYY-MM-DD],numeric value
SAS		
Precipitation timeseries	rainfall.csv	Date,rain [YYYY-MM-DD],numeric value
Evapotranspiration timeseries	evapotranspiration.csv	Date,etp [YYYY-MM-DD],numeric value

Timeseries of SAS weights	weights.csv	Date,wi [YYYY-MM-DD],numeric value

References

Grabczak, J., K. Różański, P. Maloszewski, and A. Zuber. 1984. "Estimation of the Tritium Input Function with the Aid of Stable Isotopes." *CATENA* 11 (2): 105–14. https://doi.org/10.1016/0341-8162(84)90001-8.

Maloszewski, Piotr, Werner Rauert, Peter Trimborn, Andreas Herrmann, and Rolf Rau. 1992. "Isotope Hydrological Study of Mean Transit Times in an Alpine Basin (Wimbachtal, Germany)." *Journal of Hydrology* 140 (1): 343–60. https://doi.org/10.1016/0022-1694(92)90247-S.