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D7.1: Simplified Models for WATERAGRI Innovations

Version 1*

April 2023 (M36)
WP 7 Framework Development

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Abstract:	Deliverable D7.1 “Simplified Models for WATERAGRI Innovations” describes the structure of the simplified models developed for WATERAGRI solutions. This includes the analysis and selection of the solutions and the methodology used to develop and validate the models and the current status of those under development. D7.1 is linked to Milestone M7.1 “Development of Simplified Catchment Models”.

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CI	Classified, information as referred to in Commission Decision 2001/844/EC	
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***"This is the first version of the deliverable, and it presents preliminary results as for the M36 (April 2023). The information contained in this version is subject to change, and final results will be presented in the updated version of the deliverable in M42 (October 2023). The European Commission is not responsible for any use that may be made of the information contained in this deliverable."**

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BI	Boom irrigation
CSTR	Continuously Stirred Tank Reactor
CT	Conventional tillage
CW	Constructed wetlands
DI	Drip irrigation
FC	Field capacity
FCW	Farm constructed wetlands
GNIP	Global Network of Isotopes in Precipitation
IAEA	International Atomic Energy Agency
MT	Minimal tillage
NI	No irrigation
NT	No tillage
PAW	Plant Available Water
PWP	Permanent wilting point
RT	Reduced tillage
SI	Sprinkler irrigation
TIS	Tanks-in-series model
TN	Total nitrogen
WISER	Water Isotope System for Data Analysis, Visualisation, and Electronic Retrieval
WP	Work package

1 Introduction

Managing agricultural water consumption efficiently is crucial for sustainable food production. Climate change and the ever-growing population make this task highly challenging. Additionally, nutrient availability is also becoming increasingly uncertain, and often more nutrients than the crops require are employed. This has led to diffuse contamination of water bodies through surface runoff and percolation from agricultural soils. Within this context, the WATERAGRI project aims to introduce a new framework that will help to efficiently find appropriate solutions for water and nutrient management in agricultural catchments across Europe. The project addresses three biogeographical regions of Europe (Boreal, Continental and Pannonian), and it is divided into 9 work packages (WP), each focused on a specific objective. This deliverable is part of WP7 on the Framework Development, with contributions from WP3 and WP4 on water retention, management, and nutrient recovery from streams.

Simplified models are part of the project as a decision-making tool. The solutions are tested in some case studies, where we can learn whether the solution improves water and/or nutrient management. However, it is difficult to know in advance if such a solution benefits another field, as each field has different characteristics, such as climatic conditions or soil type. Simplified models can give a glimpse of how a solution may work, providing average or approximate values. The simplified models are used to understand the effect of the solutions implemented or products applied in the field and to demonstrate how to use a solution according to the field-specific characteristics. WATERAGRI deliverable 7.1 aims to describe the simplified models built for the project's solutions.

Simplified models come in different forms and structures. The term "simplified model" refers to conceptualising a system that preserves all its essential characteristics but simplifies the representation of the physical processes. For example, rather than simulating the spatial distribution of given parameters, a simplified model provides bulk estimates representing the system average.

This document is version 1 of D7.1 Simplified Models for WATERAGRI Innovations because further information is required on some solutions to build the models. After summer 2023, this document will be updated with D7.1 (version 2). The solutions with a simplified model already developed have sections for *Model structure* and *Model validation*. Solutions for which a simplified model has not yet been built have a section for *Current status*, which will be presented in more detail in version 2. Solutions already implemented in the Framework or with a model demo are included in Section 4, *Implementation in the Framework*.

2 Analysis and selection of solutions

WATERAGRI offers a variety of solutions with different purposes that rely on different types of data. Some solutions are technologies or products that can be implemented in the field or applied directly to the soil. Others are used to gather information about the catchment to support water and nutrients management.

During the development of the solutions, clusters of solutions were identified for which we could not develop simplified models. These solutions are classified as follows:

1. **Not applicable**: A simplified model cannot be built for these solutions because they are a complex model, tool, data collection method or web platform.
2. **In the development phase**: It includes solutions that are not yet implemented on the ground on a real scale; thus, detailed technical information is not yet available. The solutions in this classification have been tested only in the laboratory or have been tested in the field, but further tests are ongoing to improve their effectiveness.
3. **Already simplified**: The solutions under this classification are inherently a simplification.

A **simplified model** for solutions that did not fall under any of the above classifications has been tested and implemented in the Modelling Framework. The solutions in the development phase will have sufficient results after the summer of 2023, and a simplified model will then be developed and implemented in the Framework. These solutions will, in any case, be provided with informative fact sheets.

The WATERAGRI solutions are presented in Table 1 along with their corresponding classification. The solutions in Table 1 are listed using the same terminology as in the Factsheets, which differs from the original project proposal. This is due to a readjustment of the nomenclature to better express the project's outcome. For example, solutions such as Remote sensing pipeline (B2), Irrigation management, and agrometeorological monitoring (B3) are merged and fully implemented in the decision-support system as the Irrigation Management Platform.

In addition to the project solutions, the DRAINMOD software has also been tested in Case Study Finland II to study the impact of drainage and water table regulations. The results are summarised in section 3.5.

Table 1: List of solutions classified according to their suitability for building a simplified model. The solutions are named as in the factsheets, and the numbering represents the solutions in the proposal.

Solutions/methods	**Not applicable**	**In development phase**	**Already simplified**	**Simplified Model within WATERAGRI**
Framework (**A1**; UNINE)	X			
Data assimilation (**A2**; FZJ)	X			
Decision support system (**A3**; AGRICOLUS)	X			
Water Retention Characteristics (**A4**, **B8,** USAL)			X	
AgriLemma Serious Game (**A6**, TUDELFT)	X			
Farm-constructed wetlands for water retention (**B1**; ULUND)				X
Remotely Sensed Data (**B2**; VULTUS)	X			
Irrigation management platform (**A5, B3, B4**; AGRICOLUS)			X	
*Water Retainer (**B5**, BZN)*		X		
Biochar for water retention (**B6**; ALCN)				X
Tracer Methods (**B7**; BOKU)				X
Farm-constructed wetlands for nutrient retention (**C1**; ULUND)				X
Filter drain pipe (**C2, C4**; ALCN)		X		
Multi-layer filter system (**C2, B6, C4**; ALCN)		X		
Biomembranes (**C3**; VTT)		X		
Microfluidic (**C5**; EDEN)		X		

3 Simplified model approach

3.1 Farm Constructed Wetlands

3.1.1 Background

Agricultural runoff is composed of nutrients, suspended solids and chemicals used in agriculture, e.g. pesticides. It contributes to diffuse pollution, which is generated from several uncontrolled sources in a catchment which individually do not pose a problem but together can have a significant impact on the environment. The nutrients that cause the most pollution by diffusion from agricultural fields are nitrogen and phosphorus compounds.

Constructed wetlands (CWs) are used to reduce the pollution load of runoff water, recover nutrients and store water in agricultural fields. Constructed wetlands (CWs) are engineered systems that mimic the purification processes of natural wetlands. They can be modified according to the processes to be enhanced, which has led to different types of CWs. In the context of WATERAGRI, we use the term Farm Constructed Wetlands (FCW) to refer to free water surface wetlands, also known as surface flow constructed wetlands. In FCWs, water flows freely over the surface and provides enough space to store water and buffer runoff events, thus being very effective in dealing with agricultural runoff. Furthermore, soil water content in their vicinity increases, and they create new habitats which are beneficial for flora and fauna.

Nitrogen removal in FCW wetlands can occur through various physical, chemical, and biological processes. Some key processes involved in nitrogen removal include sedimentation, adsorption, plant uptake and nitrification-denitrification, the latter being the most influential. In FCW, aerobic and anoxic conditions coexist. This provides a suitable environment for establishing microbes involved in nitrification-denitrification processes, which can remove up to 50% of total nitrogen (TN) (Dotro et al., 2017). As for phosphate, only 10-20% of phosphorus can be removed, decreasing removal efficiency over time. Moreover, as phosphorus is mainly retained in the sediment, the outflow concentration can be higher than the inflow concentration if it is flushed out during a runoff event. Consequently, the simplified model was built to model only TN degradation.

To find the best model configuration, we compared different simple models for water and solutes transport and nitrogen degradation under steady- and unsteady-state conditions. The data used to test the model was from a full-scale FCW located in the experimental farm of the Canale Emilio Romagnolo (CER) Land Reclamation Consortium in the Emilia-Romagna region, Italy (Case study 9 – Bologna). The FCW was 470 m long and about 8 m wide, folded by four meanders over an area of 0.4 ha. The wetland has been running and monitored for more than 20 years by the project partners UNIBO and CER. The extensive dataset and a tracer test conducted in 2017 provided the necessary data to test the models (Lavrnic et al., 2020a; 2020b). From the dataset, two runoff events of different hydraulic characteristics were selected. Event 1 had continuous inflow and outflow, and when the event started, the water level in the wetland was 10 cm. Event 2, by contrast, had discontinuous inflow and outflow and no water at the beginning of the event.

The models developed are derived from models applied in chemical and civil engineering to predict chemical reactors' behaviour and optimise their design. Therefore, we refer in the models to tanks, which represent the wetland. The transport models compared were:

- Continuously stirred tank reactor (CSTR): Assumes instant and complete mixing in a single tank, which means that the outflow concentration is equal to the concentration within the reactor (Levenspiel, 1999).
- Plug-flow with dispersion model: It simulates water transport and reactions in continuous, flowing systems under steady-state conditions. We also accounted for dispersion and used it for unsteady-state conditions, changing the hydraulic retention time (Bodin et al., 2012).
- Tanks-in-series model (TIS): This model is a CSTR train where there is complete mixing in each tank, and the water leaving one tank enters another (Fogler, 2016).

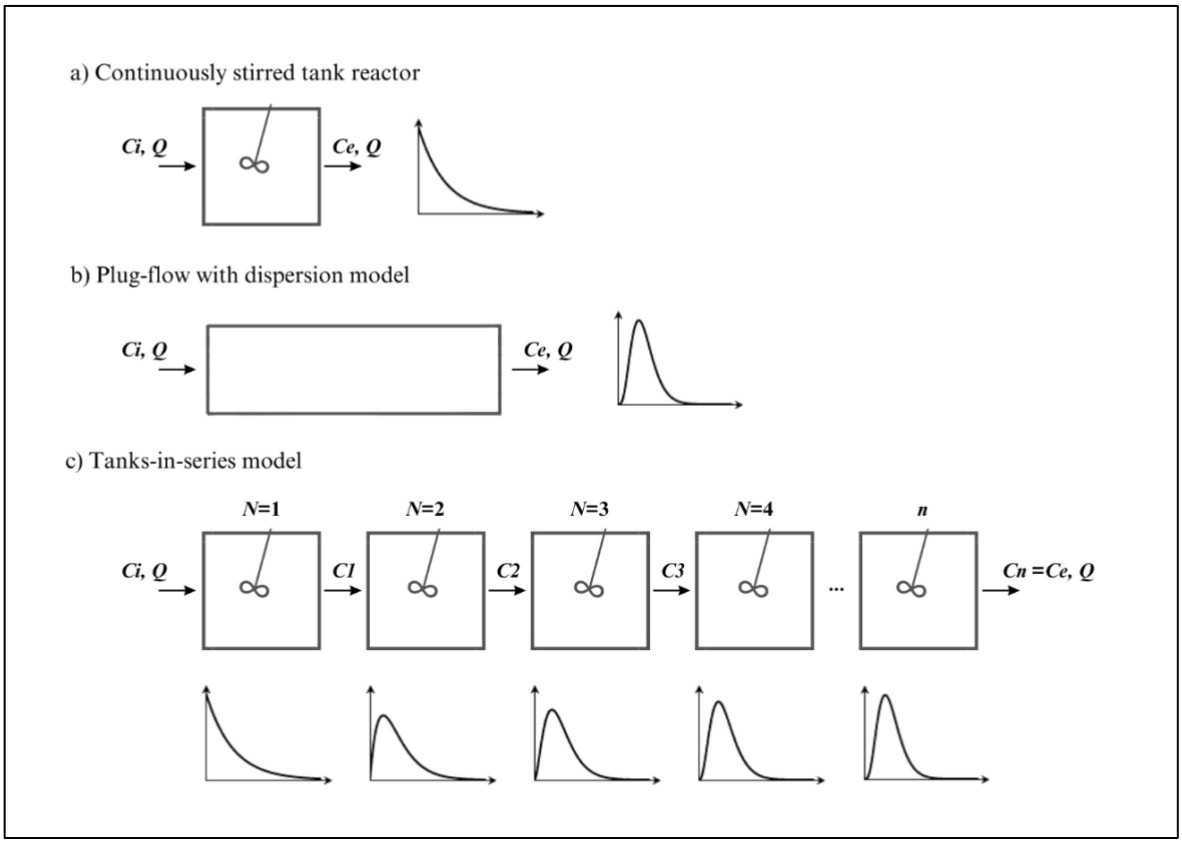


Figure 1: Transport models compared in the study. Ci and Ce are influent and effluent concentrations, Q is the inflow, and N is the number of tanks in series. In the tanks-in-series model, the Ce concentration of one tank is the influent concentration of the next tank. The curves indicate the tracer signal observed at the end of each represented tank.

The degradation models for nitrogen removal were:

- First-order kinetics: The reaction rate coefficient *k* determines the rate of the reaction, which depends linearly on the pollutant concentration.
- First-order kinetics with non-zero background concentration: Same as first-order kinetics, but it starts from a non-zero concentration, and the concentration in the tank can never fall below this threshold (Kadlec & Wallace, 2009).
- Monod kinetics: Monod equation is a model to simulate the growth of microorganisms consisting of a non-linear growth equation with a limitation, such as a lack of oxygen that would cause the reaction to slow down rapidly to a halt (Gujer, 2008).

Arrhenius equation was used to model the effect of temperature in the degradation models. For the flow conditions, steady and unsteady-state conditions were modelled to test whether the characteristics of an event influenced the performance of the model. Detailed information on this study can be found in Canet-Martí et al. (2022).

Regarding transport, the **tanks-in-series model** proved to be the most robust under **steady conditions** compared to other models. A **first-order kinetics** model **with a non-zero background concentration** provided the most accurate model for TN removal compared to other degradation models. This combination of models simulated the performance of the FCW during the two events in an hourly time discretisation, demonstrating their potential for wetland design.

3.1.2 Model structure

For design purposes, average values of outflow TN concentration and removal efficiency are calculated. Since the removal efficiency is temperature-dependent, the model takes average temperature values for each month. The model is based on the N-k-C* model (Kadlec & Wallace, 2009; von Sperling et al., 2023):

$$\left(\frac{C_e - C^*}{C_i - C^*}\right) = \frac{1}{(1 + k_v \cdot \tau / N)^N} \qquad [1]$$

where C_e and C_i are effluent and influent concentrations [g/m^3], C^* is background concentration in the FCW [g/m^3], N is a hydraulic parameter that models the apparent number of TIS, τ is mean detention time [d], also known as retention time or residence time, and k_v is the removal volumetric rate constant [d^{-1}]

The mean detention time is dependent on the area A [cm^2], the water level h [cm], inflow Q [m^3/d] and the effective volume ratio e_v [-]:

$$\tau = \frac{A \cdot h}{Q} \cdot e_v \qquad [2]$$

The effective volume ratio is used to include the effective area that is likely to be involved in the nutrient removal, as there are often dry or densely vegetated zones and stagnant zones where water flows very slowly or does not flow at all. The first order areal constant k_a [m/d] is converted into a volumetric rate constant ():

$$k_v = \frac{k_a}{e_v \cdot h} \qquad [3]$$

To consider temperature effects on the removal rate constant, a modified Arrhenius equation is included with a temperature correction factor (θ)[-]:

$$k = k_{20} \cdot \theta^{(T-20)} \qquad [4]$$

where k_{20} is the rate constant at 20°C and T is the temperature. The resulting equation estimates the effluent concentration of total nitrogen:

$$C_e = \frac{C_i - C^*}{(1 + \frac{k_{20} \cdot \theta^{(T-20)}}{h \cdot e_v} \cdot \frac{\tau}{N})^N} + C^* \qquad [5]$$

Table 2 shows the typical values of the parameters (Kadlec and Wallace, 2009) in the model and the values chosen. Influent concentration C_i, temperature T and influent Q will have a wider range and depend on climatic conditions.

Table 2: Parameters of the model with typical values and value used in the model implemented in the WATERAGRI Framework.

Parameter	Name	Units	Typical values	Value
C^*	Background concentration	mg/l	1.5 – 8	1.5
N	Number of Tanks-in-series	-	3 - 14	3
τ	Detention time	d	4 - 15	4.38
h	Water depth	m	0.4 – 1.5	0.5
e_v	Wetland volumetric efficiency	-	0.65 – 0.75	0.7
k_{20}	First order areal constant (at 20°C)	m/d	0.059	0.059
θ	Temperature correction factor	-	1.056	1.056

3.1.3 Model validation

The model is currently being validated using data on different FWS wetland performances treating agricultural runoff from Rizzo et al. (2023). Specific references with information about the wetland hydraulics will be compared to find the best fit for the number of tanks-in-series N and the removal volumetric rate constant k_v, following the methodology used in von Sperling et al. (2023) on horizontal flow wetlands.

3.2 Tracer methods

3.2.1 Background

Tracer techniques are commonly used for studying hydrological processes, such as water movement through the hydrological cycle and groundwater recharge (Leibundgut et al., 2009). Among tracer methods, isotope techniques play an important role. In the WATERAGRI project, we used the isotopic composition of precipitation water to understand hydrological processes in agricultural soils. This information can greatly assist in adapting practices to maximise resource use.

Precipitation water contains stable isotopes of hydrogen and oxygen, namely deuterium (^2H) and oxygen-18 (^{18}O). The relative abundance of these isotopes compared to the most common forms of hydrogen and oxygen (^1H and ^{16}O) provide information about different processes (Leibundgut et al., 2009; Cook, 2020). These relative abundances are expressed as water stable isotope ratios ($\delta^{18}O$ and δ^2H). The isotopic composition of precipitation water varies depending on a number of factors, including temperature, altitude, and the source of the moisture. By analysing the isotopic composition of precipitation water, it is possible to determine the origin of the moisture and to track the movement of water through the hydrological cycle. For example, water that has evaporated from the ocean has a different isotopic signature than water that has evaporated from continental surfaces such as lakes or rivers. This allows researchers to distinguish between different sources of moisture and to track the movement of water from one location to another.

In addition to tracking water movement through the hydrological cycle, the isotopic composition of precipitation water and soil water can also be used to estimate soil water fluxes, e.g. mobile soil water and groundwater recharge. Different isotopic signatures in precipitation water can be observed over the year, producing a seasonal and geographical distribution that generates a global distribution map (Rozanski et al., 1992). The seasonal variations may still be observed in the water of a soil profile, with an attenuation of the signal depending on transport processes (i.e. dispersion and diffusion). Thus, the measurement of $\delta^{18}O$ and $\delta^{2}H$ in pore water allows tracking water from different precipitation events in the unsaturated zone to provide integrative information about sources, flow, and water transport in large scales and long time-series (Stumpp et al., 2018).

This simple model is known as the peak-shift method. This technique uses **water stable isotopes** to **quantify soil water fluxes** (Barbecot et al., 2018; Chesnaux and Stumpp, 2018). This method involves analysing water stable isotopes and soil water content in the soil profile to identify the **seasonal isotopic signature of precipitation water in the soil profile**. As the precipitation water moves through the soil, it pushes old water downwards. Thus, the method assumes a predominantly convective flow in a vertically downward direction. The method relies on the principle that water fluxes with different velocities will reach different depths in the soil profile. Additional hydrological processes, such as evapotranspiration, can be quantified using the water balance approach (Boumaiza et al., 2020, 2021). More information on the application of the method can be found in Barbecot et al. (2018), Chesnaux and Stumpp (2018) and Leibundgut et al. (2009).

3.2.2 Model structure

To understand the model structure, it is necessary to know the steps followed to gather the required data and quantify soil water flux (Figure 2). The proposed simplified model uses the amount and isotopic composition of soil water and precipitation as follows:

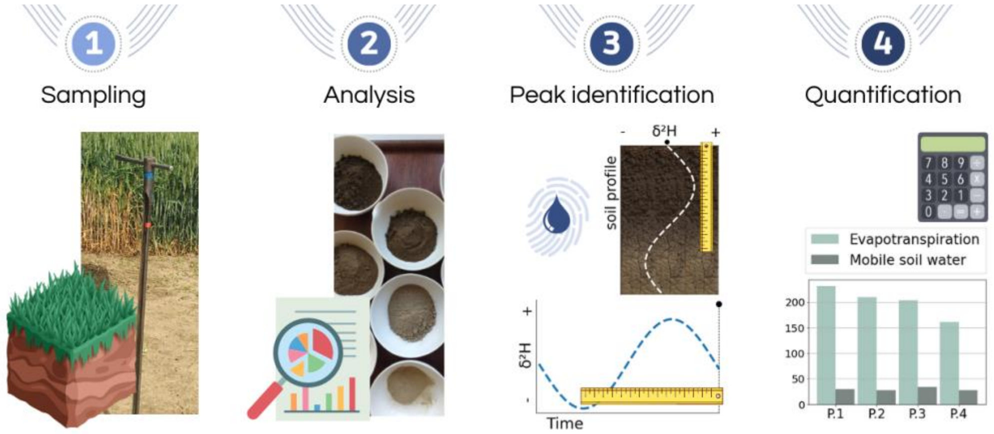


Figure 2: Steps of the tracer method to quantify average soil water flux and hydrological processes.

1. **Sampling**: Sampling soil core samples with a soil auger to a minimum depth of 100 cm. The sampling is done by sub-intervals between 5 and 10 cm and stored in sealable, inflatable and leak-tight bags (e.g. Ziploc® bag or laminated Aluminum-bags).
2. **Analysis**: Determination of the isotopic composition of pore water and volumetric or gravimetric water content (θ_w, in cm^3/cm^3; θ_g, in g/g) of soil samples.

3. **Peak identification**:
    a. Comparison of the temporal variation of (1) isotopic composition of soil water along the soil profile with (2) isotopic composition of precipitation water prior to sampling.
        i. Isotopic composition of precipitation can be obtained from in situ measurements, available open access data such as the WISER portal (GNIP-IAEA; https://www.iaea.org/services/networks/gnip) , or predicted monthly time series of $\delta^{18}O$ and $\delta^{2}H$ (available in: https://isotope.bot.unibas.ch/PisoAI/) (Nelson et al., 2021)
    b. Identification of a common period or peak/nadir. Definition of a soil Interval ($\Delta z = z_{t+T} - z_t$) corresponding to a period of time *P*.
4. **Quantification**:
    a. If only gravimetric water content is available, it has to be converted into the volumetric water content using the soil bulk density (ρ_b), if known or an approximation depending on the soil type (Eq. 6; Table 3).

$$\theta_w = \theta_g * \rho_b \qquad [6]$$

    b. Based on the soil type, residual water content (θ_r) can also be estimated (Table 4).
    c. Soil mobile water quantification: Sum of the volumetric water content of each subsample minus the residual water content ($\theta_w - \theta_r$) for the identified soil interval ($z_{t+T} - z_t$), in mm, divided by the period *P*, in yr [Eq.7].

$$q_{(z,T)} = \frac{1}{P}\sum_{i=0}^{m}(\theta_w - \theta_r)(z_{i+1} - z_i) \qquad [7]$$

The soil water flux $q_{(z,T)}$ is considered potential groundwater recharge or mobile soil water if the soil interval is still within the root zone. This information can be included in a water balance to estimate other hydrological fluxes in the agricultural field.

Table 3: Most frequent values for bulk density in soils. Data from Hartge and Horn (1999)

Textual Classes	Bulk Density, ρ_b [g/cm^3]
Clay soils	1.32 – 0.92
Silty soils	1.53 – 1.19
Loamy soils	1.96 – 1.19
Sandy soils	1.67 – 1.19
Organic soils	0.48 – 0.12

Table 4: Residual water content (θr) estimated using the Rosetta model for different textual classes (Schaap et al., 2001)

Textual Classes	Residual water content, θr

	(cm^3/cm^3)
Silty Clay	0.070
Silty Clay Loam	0.089
Sandy Clay	0.100
Clay	0.068
Silt	0.034
Clay Loam	0.095
Silt Loam	0.067
Sandy Clay Loam	0.100
Loam	0.078
Sandy Loam	0.065
Loamy Sand	0.057
Sand	0.045

Example of quantification:

- Soil core samples are taken in mid-June.
- A winter minimum in the isotopic composition is identified at 30 cm depth.
- The winter minimum is precipitation from December of the previous year, i.e. period $P \approx 6$ months.
- A sum of the volumetric water content using Eq [7] (subtracting the residual water content) of the first 30 cm (e.g. 46 mm).
- Potential groundwater recharge or soil mobile water = 46 mm /6 months = 7.6 mm/month = 92 mm/yr.

3.2.3 Model validation

3.2.3.1 Application in Case Study 8 – Obersiebenbrunn (Austria)

The simplified approach was tested in an agricultural field with different management practices (i.e. soil tillage practices and irrigation systems). The field was located in Obersiebenbrunn (Lower Austria, Austria), in an experimental field owned by the Obersiebenbrunn Agricultural School and managed with BOKU to research and train new farmers. The field was divided into sixteen plots to cover all combinations of four tillage variants and four irrigation systems. The tillage practices compared were conventional tillage (CT), reduced tillage (RT), minimal tillage (MT) and no tillage (NT), and the irrigation systems were boom irrigation with nozzles (BI), sprinkler irrigation (SI), drip irrigation (DI) and no irrigation (NI).

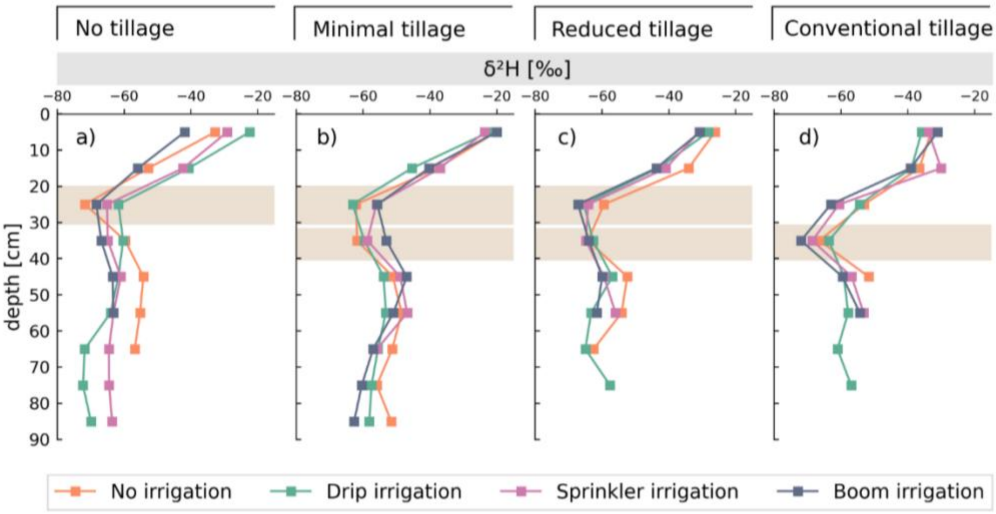


Figure 3: Profiles of isotope ratio of deuterium (δ²H) (‰) of each soil profile for each tillage variant and irrigation systems. The shaded area indicates the depth where the winter minimum was identified. Adapted from Canet-Martí et al. (2023).

At the end of May 2020, soil samples were taken from all the plots down to 90 cm depth every 10 cm (n=144). The isotopic composition of soil samples was analysed, and the δ^2H profile was compared with the δ^2H pattern in precipitation water to identify the temporal interval in the soil profile. In the soil profiles, precipitation water from the end of November 2019 shaped a winter minimum, i.e. precipitation significantly depleted in heavy isotopes, between 20 and 40 cm depth, representing 6 months of precipitation. Soil water content was determined from the same soil samples. Eq [7] was used to quantify soil water flux from the soil water content in the soil interval identified. In addition, evapotranspiration was estimated using a soil water balance approach. In the water balance, soil water flux was considered mobile soil water because the flux was calculated within the root zone, i.e. maximum root depth between 150 and 180 cm.

The method was successfully applied to quantify the average water flux in all the plots, which ranged from 3.8 to 7.6 mm/month, with differences among the treatments. Mobile soil water ranged from 23 to 46 mm, and cumulative evapotranspiration ranged from 146 to 244 mm for six months. The soil isotope profiles showed a clear difference in flow velocity between the tillage variants. The winter minimum was located deeper in the soils managed under CT (35 cm), indicating a higher water flow velocity than the rest of the tillage variants. NT soils had the lowest water flow velocity, with the winter minimum located at 25 cm depth. The reduced and minimal tillage practices showed intermediate flow velocities. No differences in water flow velocity were observed between the irrigation systems. The increase in tillage intensity showed clear trends for evapotranspiration and mobile soil water; the more intensive the tillage, the higher the evapotranspiration and the lower the mobile soil water. As for irrigation systems, irrigation water contributed mostly to evapotranspiration. SI contributed significantly to evapotranspiration, while NI contributed the least to evapotranspiration.

In conclusion, the method allowed direct quantification of average water flux in a given period. It could compare the influence of different field management practices on hydrological processes in a single sampling campaign, as the stable isotopes of water in the soil profile may provide information for several months. The study results are presented in Canet-Martí et al. (2023) and deliverable 3.2 on Assessment of Water Retention Methods.

3.2.3.2 Scenarios testing: A simulation study

Soil hydraulic properties and climate influence the soil water isotopic signal. Some soil characteristics can influence the attenuation of this signal, such as soil dispersivity or soil texture. On the other hand, the precipitation pattern, the amplitude of winter and summer temperatures or continentality can affect the identification of a peak or nadir in the soil. Numerical modelling has proven to be a valuable tool for the study of water flux and solute transport in the vadose zone. In this regard, the hydrological model HYDRUS-1D has already implemented a modification to simulate isotope transport that accounts for evaporation fractionation (Stumpp et al., 2012; Zhou et al., 2021).

HYDRUS is a finite element model for simulating water flow, solute transport and heat in one-, two- and three-dimensional variably-saturated porous media. HYDRUS solves Richards equation to describe water flow and advection-dispersion type equations for heat and solute transport. The isotopes module modifies the input function of the solute transport module to simulate the fate and transport of stable water isotopes ($\delta^{18}O$, $\delta^{2}H$) (Stumpp et al., 2012). It assumes that fractionation processes can be neglected, and the isotopes do not accumulate at the upper boundary due to evaporation as solutes do.

This study used seasonal isotopic signals representative of three biogeographical regions (i.e. Pannonian, Continental and Boreal) as input signal in HYDRUS-1D. The climate scenarios were tested using soil textual classes and longitudinal dispersitivies (Table 1Table 5). The results provide an overview of the characteristics of the soil in which the isotopic signal could be observed for subsequent quantification of soil water flux (Figure 4). The aim was to provide sampling recommendations, such as the best time for sampling and appropriate depth intervals for sampling. So far, the profiles generated for a scenario in Vienna show soil isotope profiles consistent with our study in Obersiebenbrunn.

Table 5: Biogeographical regions, soil textual classes and longitudinal dispersivities that compose the simulation scenarios

Biogeographical regions	Textual Classes	Longitudinal dispersivity, D_L [cm]
Pannonian	Clay	1
Continental	Clay Loam	5
Boreal	Loam	10
	Loamy Sand	20
	Sand	
	Sandy Clay	
	Sandy Clay Loam	
	Sandy Loam	
	Silt	
	Silty Clay	
	Silty Clay Loam	
	Silty Loam	

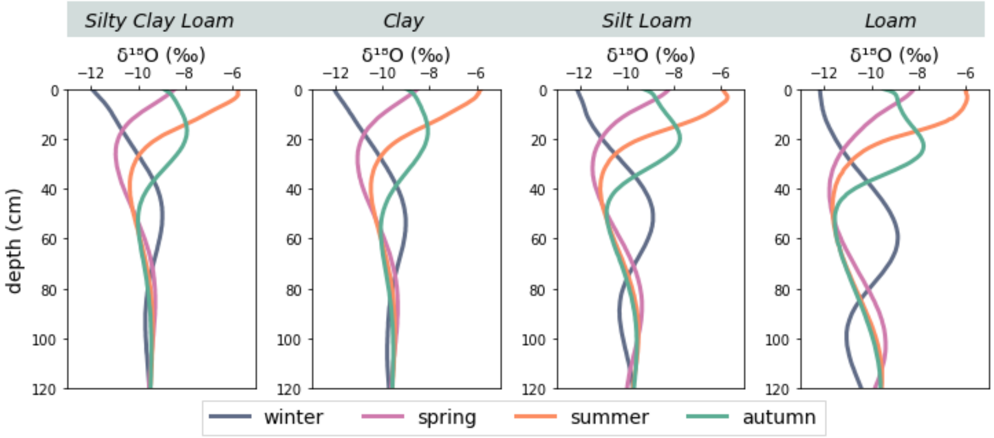


Figure 4: Simulated $\delta^{18}O$ contents of soil water to a depth of 120 cm for different soil textures in Vienna (Longitudinal Dispersivity = 1cm)

3.3 Biochar for water retention

3.3.1 Background

Biochar is a type of charcoal produced by heating organic matter in the absence of oxygen. When added to soil, biochar can have a range of beneficial effects on soil properties, including water retention. The impact of biochar on water retention in soils depends on several factors, including the type and amount of biochar used, soil properties, and environmental conditions. In general, biochar can improve water retention in sandy soils by increasing the soil's ability to hold onto water, while in clay soils, it can improve drainage by creating channels for water to move through (Abel et al., 2013; Razzaghi et al., 2020). Similarly, adding biochar increases saturated hydraulic conductivity in clay soils while decreasing it in sandy soils (Lim et al., 2016; Edeh et al., 2020).

During the last decade, many related research studies have used field-scale experiments or laboratory studies analysing changes in the water retention curve and simulation studies with complex models, e.g. HYDRUS model (Wu et al., 2019; Dokoohaki et al., 2017). These tools can help researchers and practitioners evaluate the effectiveness of biochar in improving soil water availability and identify the most appropriate application rates and methods for different soil types and environmental conditions. However, using these tools takes time and a certain degree of experience. Therefore, we have compiled information from studies to create a simpler model that can serve as a guide to determine the effect of adding biochar on soil water retention. Among the studies included, we highlight the review studies carried out by Lim et al. (2016) and Razzaghi et al. (2020).

Predictive tools for water retention in soils with added biochar can help to guide the development and implementation of biochar applications for improving soil water availability. However, it is important to note that the effectiveness of biochar in improving soil water retention may vary depending on environmental conditions and the ageing of the biochar as it changes its properties (Edeh et al., 2020).

3.3.2 Current status

To build up the model, we analysed information gathered from research and review papers. The resulting database gathers information on changes in the water retention curve for different biochar application rates in different soil textures. The water retention curve provides information on the water content at field capacity (FC) and water content at the permanent wilting point (PWP). The plant available water (PAW) is equal to FC minus PWP. The change in PAW enables us to calculate the percentage change (increase or decrease) in water availability in different soils as a function of biochar application rate.

The simplified model will be verified with an experiment carried out in the soil physics laboratory of BOKU, where two biochars with different particle size distribution will be added to two soil textures with different application rates. The study will evaluate changes in the water retention curve, saturated hydraulic conductivity, and bulk density. It will be conducted between March and June 2023.

3.4 Biochar for drainage water treatment

3.4.1 Background

Nutrients removal by biochar depends on biochar characteristics and the compounds present in the water. Although some authors have highlighted the potential of unmodified biochar to remove nitrogen and phosphorus compounds by adsorption, it has been shown that the adsorption capacity of biochar to remove ammonium, nitrate, and phosphate is relatively low (Zhang et al., 2020). For example, the negatively charged surface of biochar repels nitrate and phosphate ions. To overcome this limitation, biochar chemically modified with metals has been used for the drainage filter in Case Study 8.3 (Gleisdorf, Austria). Modified biochar has shown higher removal efficiency for all nutrients compared to non-modified biochar (Zhang et al., 2020). That is the case of Mg-coated biochar, which triggers the precipitation of phosphate and, if phosphate concentration in the biochar is high, also of ammonium, forming struvite (Fan et al., 2019).

In Case Study 8.3, a filter structure was adapted and placed at the end of a subsurface drainage pipe from sloped organic farmland. After three trial experiments to find the best configuration, the filter structure was composed of two cartridges of 70 cm long, each with a volume capacity of 8 L. One cartridge was filled with $Mg(OH)_2$-coated biochar from cherry seeds and the other one with zeolite (4-8 mm). The combination showed good hydraulic performance and the potential to remove phosphate and nitrate from agricultural runoff. However, there were not enough rain events to test the system during the first monitoring year (2022). Detailed information on the structure configuration and the results are reported in Deliverable 4.3 Description of developed Drainage Technologies, and in the factsheet for “filter drain pipe”.

3.4.2 Current status

Currently, a laboratory experiment is being carried out to test both filters ($Mg(OH)_2$-coated biochar and zeolite) to better understand the contribution of each material to nutrients removal under three different flow rates. The concentration in the inlet will be the same during the whole experiment with artificial agricultural runoff water. The results will help compile data to build a simplified model and give recommendations to support the design of filters for the treatment of drainage water using biochar.

3.5 DRAINMOD

3.5.1 Background

DRAINMOD 6.0 is a computer program that simulates the hydrology, water quality, and crop growth of agricultural drainage systems. It is a tool for predicting the effects of agricultural practices, weather, and soil properties on water quantity and quality, crop yields, and nutrient losses from drained fields. Researchers, consultants, and farmers use DRAINMOD 6.0 to evaluate the performance of drainage systems, design drainage systems, and develop management strategies for sustainable agriculture. It is a powerful tool for assessing the environmental impact of agricultural activities and for optimising agricultural production while minimising negative effects on water resources. In WATERAGRI, it is used to study the impacts of drainage and water table regulations.

3.5.2 Model structure

The structure of DRAINMOD 6.0 consists of three main components: a hydrologic model, a soil water balance model, and a crop growth model. Together, these models provide a comprehensive simulation of the hydrology, water quality, and crop growth of agricultural drainage systems. The model can be used to evaluate the effects of different drainage and water table management strategies on water resources, crop production, and nutrient losses. We used the first two models because the purpose of the study was to observe the drainage and water table regulation.

- The **hydrologic model** simulates the water movement within the soil profile and the drainage system, considering the effects of precipitation, evapotranspiration, soil properties, and drainage characteristics. It predicts the rate and timing of water movement into and out of the soil profile and the drainage system.
- The **soil water balance model** calculates the water balance of the soil profile, including the changes in soil water content due to infiltration, evapotranspiration, drainage, and runoff. It also predicts the water table depth and the hydraulic conductivity of the soil.

3.5.3 Model validation

DRAINMOD software was built and calibrated to all 6 field blocks in the Ruukki site, Finland. The model was run for three years data from the site and in-situ measured meteorological, hydrological, and soil parameters were used in the model in daily timestep. Meteorological data included precipitation, temperature and other relevant parameters. Ruukki site hydrological parameters used in the model included groundwater table, soil moisture and discharge from the sub-drainage system. DRAINMOD was mainly calibrated against the groundwater table in each 6 field blocks. Soil parameters used in the model included pF curve (water retention), soil hydraulic conductivity, soil type and layers. The model was successfully built, but calibration was challenging to include daily temporal variation. The model produced monthly groundwater table levels but failed to produce daily temporal variation, which would be essential information for managing sub-drainage or sub-irrigation systems.

Main results:

- DRAINMOD was able to predict the annual and monthly water tables but failed to produce a dynamical function of the water table variation on a daily level.
- The problem of including the regional main drainage system in the model was the main challenge in DRAINMOD calibration.

- Ruukki fields are surrounded by large open ditches that influence groundwater levels in the field, and this additional drainage influence was not successfully implemented in the DRAINMOD model.
- Solutions would be to use a three-dimensional model that can also include influence on the regional drainage systems, not only field-based drainage systems, to the numerical model.

DRAINMOD modelling is unsuitable for cultivated peatland sites with controlled drainage if the studied area is influenced by large open drains.

4 Implementation in the Framework

4.1 Farm Constructed Wetlands

4.1.1 Input and output data

The simplified model for FCWs aims to indicate what the total nitrogen removal efficiency of an FCW would depend on the characteristics of the input water (i.e. concentration and flow) and the size and shape of the wetland at the site where it is to be constructed. The removal efficiency is strongly influenced by temperature. Bacteria that carry out nitrification-denitrification processes grow better at higher temperatures, so the efficiency will be higher in summer. This is represented in the model with average efficiencies calculated from the local monthly average temperatures.

The volume of the wetland will also influence the amount of water that can be stored in the wetland and will contribute to a higher soil water content around the wetland, as well as storing water from heavy rainfall events for its use in times of water need.

The model inputs filled in by the user are:

- Geographic Location
- Inflow (Q) in m^3/d
- The influent concentration of total nitrogen (Ci) in mg/L
- Wetland area (A), in m^2
- Background concentration of Total Nitrogen (Cb) in mg/L
    - Low: 1.5 mg/L
    - Medium: 3.5 mg/L
    - High: 8 mg/L
- Number of Tanks in series (*N* or P), which depends on the shape of the wetland. The range goes from 1 (square FCW) to 14 (very long).

The user can change the parameters Q, Ci, A, Cb and *N* to find out how the quantity and quality of the influent runoff water and the configuration of the wetland will affect its performance. Cb and *N* have ranges, while Q, Ci and A are user-dependent. The minimum Cb is 1.5 mg/L because the concentration cannot be as low as 0 mg/L. Cb of up to 8 mg/L is common and even higher in more extreme cases. As for *N*, the minimum is 1, representing a squared wetland (Figure 1), while an *N* greater than 14 would not affect the treatment. The user will get information on how to calculate Q and what typical ranges of Ci can be found in agricultural runoff water.

Regarding the surface area (A), the optimal solution is to find an area large enough to treat the runoff water that does not require too much space in the field. The efficiency of the treatment will reach a limit where even if we increase A, the efficiency will not increase, as it is limited by Cb and the air temperature.

4.1.2 User interface

1. First, the user can select the field directly from the map or enter the address in the upper right corner to locate where the FCW would be constructed.

Figure 5: Screenshot of the map where the user can locate the farm-constructed wetland.

From the geographic location chosen by the user, an API call is made to the weather data provider MeteoStat, and all monthly average temperatures from 2000 to 2020 are downloaded.

2. By obtaining the average monthly temperatures, the model directly calculates the total nitrogen concentration at the wetland outlet (C out) in mg/L and the removal efficiency in % (shown in the table) from the pre-determined parameters (displayed below the table).

Month	Temperature (°C)	C out (mg/l)	Removal efficiency %
January	4	17	24 %
February	5.3	16.7	25 %
March	9	15.7	30 %
April	12.6	14.7	34 %
May	17.2	13.2	41 %
June	21.4	11.8	47 %
July	23.8	10.9	51 %
August	24	10.9	51 %
September	19.6	12.4	44 %
October	15	13.9	38 %
November	9.6	15.6	30 %
December	4.8	16.8	25 %

Inflow (Q) 80 m^3/d

Inlet concentration of Total Nitrogen (Ci) 22.3 mg/l

Area (A) 1000 m^2

Apparent number of Tanks in series (P) 3

Background concentration of Total Nitrogen (Cb) 1.5 mg/l

Figure 6: Screenshot of the user interface of the simplified model for farm-constructed wetlands. The map where the wetland is located, input variables to be changed and the table with output values from the model.

3. Finally, a graph shows the months on the horizontal axis, the temperature in °C on the left vertical axis (X1) and the output concentration in mg/L on the right vertical axis (X2). The graph and the values in the table (Cout and removal efficiency) will change automatically when the input parameters or the location of the wetland are changed.

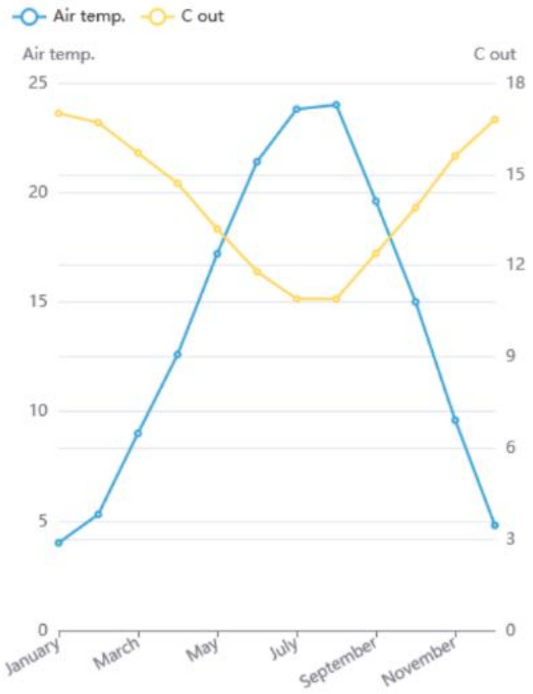


Figure 7: Graph of monthly average air temperature and total nitrogen outflow concentration in mg/L.

4. Information on the side with a description

More detailed information on the parameters, model limitations and specifications will be shown, as well as how to determine which value best represents the specific water and wetland with the appropriate units of measurement, e.g. inflow in m^3/d.

4.2 Tracer methods

4.2.1 Input and output data

The simplified model on tracer methods shows the soil isotope profile of the ($\delta^{18}O$). Through evaluation of the Oxygen isotope in the soil it is possible to track the movement of water and quantify the water flux in the soil. The main advantage of this method is the possibility to quantify water fluxes in fields that are difficult to access or have little data available by carrying out a single sampling campaign.

For visualisation, the user should select from the drop-down list the (1) climate scenario and (2) the soil texture:

- Climate scenario:
    - The scenarios result from specific locations representing all combinations of biogeographic regions (i.e. Continental, Boreal and Pannonian) and the climates of the Köppen climate classification that can be found in those regions.
- Soil texture class:

  - The user can choose between the twelve soil texture classes (USDA): sand, loamy sand, sandy loam, sandy clay loam, loam, silt loam, silt, silty clay loam, clay, clay loam, sandy clay and silty clay.

Output:

- Expected distributions of isotopic composition in soil pore water up to 200 cm depth depending on the season when the sampling campaign takes place.
- The results provide an overview of the soils characteristics in which the isotopic signal could be observed for subsequent quantification of soil water flux.
- The user will get sampling recommendations, i.e. best timing for sampling and adequate depth intervals for sampling, required minimum soil depth

4.2.2 User interface

The user interface allows users to select the soil type and climate scenario to produce a chart with water stable isotopes profiles. The colours represent the season when the samples are taken. Since precipitation water shows seasonality in its composition and the most recent water pushes the soil water downwards, depending on the sampling time, we will find minima and maxima at different depths, as shown in Figure 8.

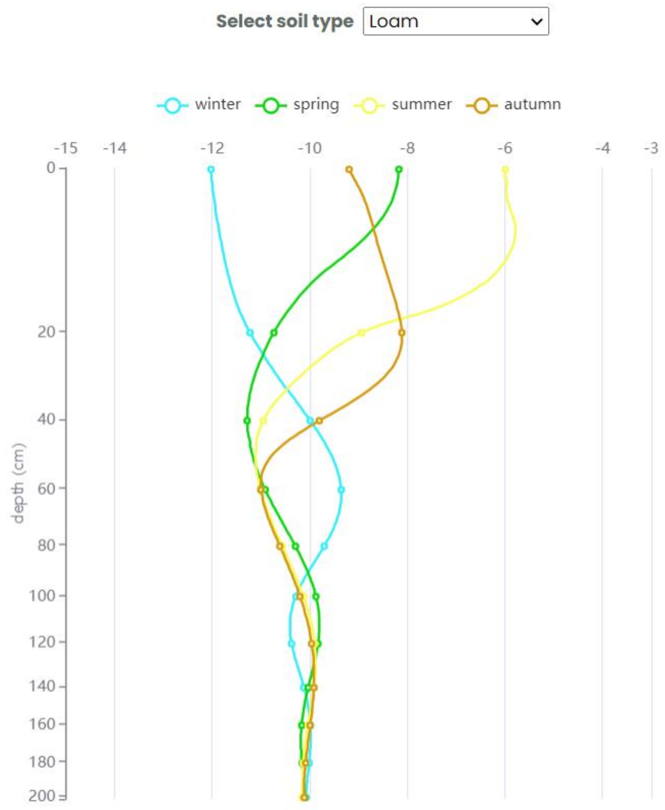

Select soil type Loam

Figure 8: Graph displayed in the user interface of the simplified model on tracer methods.

Subsequently, the user will get general information on $\delta^{18}O$ profiles and sampling recommendations:

- The $\delta^{18}O$ profiles displayed can help you identify the best sampling time based on your needs.

- Sampling should be carried out according to the information to be obtained, e.g. water flux quantification during a cropping season.
- The sharper the maximum or minimum, the better the periods can be defined.
- Conventionally tilled soils (up to 30 cm depth) may have maxima/minima at greater depths.
- Avoid sampling after a long drought to avoid confusing a summer peak with an evaporation front.
- Sample every 5 cm to locate the peak more accurately where the maxima/minima are expected, depending on the climate scenario, soil type and sampling season.
- In areas with shallow water table, this method cannot be applied.

Specific information for climate scenarios:

Example: **Continental-Marine West Coast Climate (Vienna)**

- This climate is mild, with no dry season and warm summers. In this scenario, $\delta^{18}O$ values of precipitation range from -6 to -12 ‰. This range is mainly influenced by air temperature. Precipitation $\delta^{18}O$ values are most negative in winter and least negative in summer.

And depending on the soil texture:

Example **Silt**

- In this soil type, with low clay content (<30%), the longitudinal dispersivity is typically lower, so the maxima/minima are sharper.
- Integrative information on water fluxes in the upper 70 cm at most represents the last 6-10 months if sampled in winter or autumn. At deeper layers, even more, peaks can be found.
- Take subsamples every 5 to 10 cm

Moreover, the user will also find information on the model structure and quantification, as explained in section 3.2.

4.3 Biochar for water retention

4.3.1 Input and output data

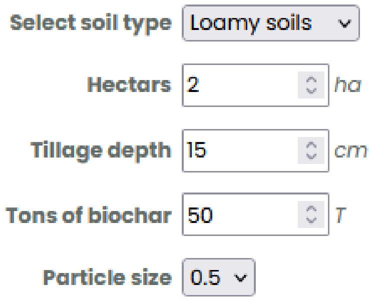
The Water Retention model using Biochar aims to indicate how much water will be saved based on particle size and the amount of Biochar. The model inputs filled in by the user are:

- **Soil texture**
- **Field hectares** where the biochar will be applied
- **Tillage depth**, in cm, is the depth to which the tillage reaches.
- **Tons of biochar** applied
- **Biochar particle sizes** (0 to 0.5 mm; 0.5 to 1mm; 1 to 2mm)

The model's output is the change in plant available water (PAW) shown in % of water per ha compared to the % of PAW in the soil without biochar.

4.3.2 User interface

The initial screen for the user shows the model inputs required to quantify PAW (Figure 9). The boxes have no default values, so the user has to fill them in from the beginning.



Select soil type Loamy soils

Hectars 2 ha

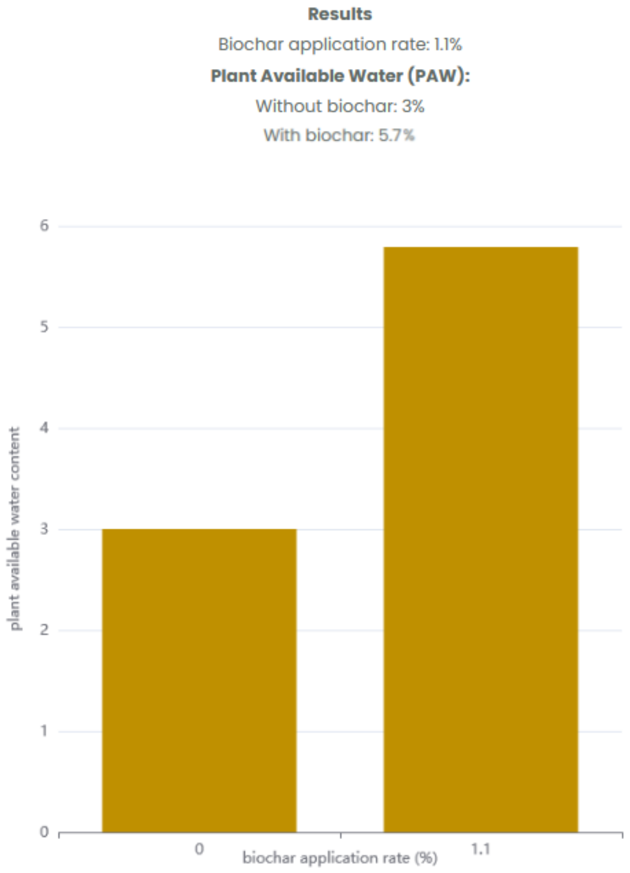
Tillage depth 15 cm

Tons of biochar 50 T

Particle size 0.5

Figure 9: User interface for the biochar for water retention model. The user finds empty values to add information on the soil type, tillage depth, hectares to apply the biochar, tons of biochar and particle size of the biochar.

The model calculates the applied biochar rate and shows the percentage of PAW for soil with and without biochar in written form and a graph so that the difference can be seen more clearly (Figure 10).



Results

Biochar application rate: 1.1%

Plant Available Water (PAW):

Without biochar: 3%

With biochar: 5.7%

Figure 10: Screenshot of the simplified model for water retention by applying biochar in the soil.

The system has been evaluated by stakeholders who provided suggestions for improving the definitions of variables. A description of the method and information on how it can be used and its limitations will also be added.

5 Conclusions

This deliverable shows the progress made so far with the simplified models and their implementation in the modelling framework of the WATERAGRI project. The first iteration of the User Interface of the simplified models has been used to gather feedback and ideas from end-users to improve it. The suggestions will be incorporated in the final version of the Visual Interface available in M45 and described by D7.4 *Visual Interface*.

The models are being extended to provide clearer information for different types of users. In addition, the models are being tested to improve their accuracy. The simplified models give average values of how these solutions could be used in different agricultural fields depending on their characteristics and climatic conditions. It is important to note that these are not models for design. The design and implementation of the solutions should be done by a professional.

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