DOCTORAL (PhD) THESIS

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Gödöllő Campus

2025

Hungarian University of Agriculture and Life Sciences

Gödöllő Campus

Spatial AquaCrop. A new tool for utilizing AquaCrop in a raster based environment

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Gödöllő

2025

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1. INTRODUCTION

Production from agriculture has been increasing for the past century, mostly due to productivity enhancing technologies and an increase in efficiency in using natural resources for the purpose of enhancing agricultural production, especially for food (FAO, 2017). Even though productivity has increased, a good and efficient management of natural resources still needs to be one of the goals of modern agriculture, especially when taking in consideration the necessity of preserving the natural environment (Pimentel et al., 1997).

Water as a natural resource is one of the most important for agriculture as it can be crucial for several reasons, some of the most important ones could be said to be increasing crop productivity, maintaining a balanced environment for the crop (Saad et al., 2020) and ensuring that these water sources do not suffer from any pollutant and are not overused some of the biggest challenges for sustainable agriculture. (Cosgrove and Loucks, 2015)

Water is a renewable resource, however due to increase of human population, water demands have continuously increased, and uneven distribution of water availability makes it even harder to meet this demand (FAO, 2023, Bennett, 2000). Water issues have then become among the top risk and one of the most important goals on the Sustainable Development Goals (FAO, 2023; UNWWDR, 2018). In the past many different decisions have been made that have not improved sustainability or security regarding water resources (Cosgrove and Loucks, 2015), this was mainly done for short term financial gains, not considering long term environmental or economical sustainability of the water resources.

The agricultural yield is directly affected by the availability of water, but not just external factors can affect negatively water availability, agriculture itself can also affect it negatively (Wats et al., 2015). Agriculture can be in many regions a major user and polluter of water as irrigated agriculture can be one of the major users of water globally (Saad et al., 2020). A proper water management is a necessity nowadays as water scarcity has become an essential topic in any discussion about crop production or field management (Letseku and Grové, 2022). It is good to take in consideration that crop yield increases with water availability that is available in the root zone of the soil, until the saturation level of it, afterwhile water availability there is not much effect to the plant yield (wu et al., 2022, Medici and Wrachien, 2016).

One important aspect of water management in agriculture is the water productivity, which is in simpler terms the value or amount of a final product, for example crop yield, in relation to the volume of water used or diverted in the process (FAOa). Crop water production is mainly affected by transpiration, but in a broader sense evapotranspiration could make more sense as it takes into consideration the whole system and not just the water transpiration by the crop (Letseku and Grové, 2022). With this aspect in mind, different tools like, modeling, spatial analysis, irrigation management and others can be used to improve water productivity and improve the efficiency of how the water is used in the agricultural system (Letseku and Grové, 2022).

Soil moisture is a key component of the hydrologic cycle and needed for a proper management of the water necessary for a crop to properly achieve its best yield (Cai et al., 2023), for that it is an important aspect of the water management in agriculture fields to be studied. Knowing the soil moisture content of a field can show how much irrigation would be needed for a crop to grow or if the irrigation that is being conducted is being excessive and wasting water. Soil moisture is extremely variable and nonlinear in space and time (Heathman et al., 2012), and it regulates interactions between the land surface and atmospheric processes (Brubaker and Entekhab, 1996). Undoubtedly, soil moisture influences how an ecosystem responds to its physical surroundings by influencing the surface energy budget and the partitioning of rainfall into runoff or infiltration (Joshi et al., 2011).

Directly measuring soil moisture and other hydrological indicators can be quite time and work intensive, for that the usage of mathematical models to predict soil moisture are more viable (Singh et al., 2023), being it as well a cost-efficient way to test reactions to agricultural systems due to external change. Nowadays there are three main approaches in measuring soil moisture, the first is using gravity surveys to take measurements in the field, enabling the usage of probes in the soil (Rasheed et al., 2022), being one of the most widely used approaches for soil moisture measurement. The second approach would be the usage of soil moisture models, which can cover a larger area than just the probes, but they are dependent on the availability of other variables such as, meteorological data, different soil and plant parameters (Chandrappa et al., 2023). The third one is remote sensing utilizing the microwave length, as it can record values anytime of the day, just being susceptible to cloud cover (Mu et al., 2022). Having a mixture of all of these 3 while analysing soil moisture or other parameters related to it can be good methodology as it uses the best points of each one of them (Singh et al., 2023).

Understanding and timely monitoring of the dynamics of soil moisture is not only critical for agricultural production, but also for nature conservation and the improvement of general welfare of the globe, for that being able to model it, to not be dependent on site measures is a good alternative. Available precision agriculure solutions (based on electrical conductivity measurements) can provide detalied, spatially explicit information of the top soil layer’s wate content (Balla et al., 2017). However, these methods alone are dependent on the timing of management practices and cannot provide timely assesment of irrigation demand. There are different types of models that can measure soil moisture, some examples are: AquaCrop (AquaCrop, 2024), Leak Bucket (Leaky bucket model, 2024), NLDAS (NLDAS, 2024), hydrus (Hydrus, 2024), BEACH (Sheikh et al., 2009), etc. Modeling provides a mathematical tool to be used to enhance how we can optimize the water usage in cropping systems (Kisekka et al., 2017).

AquaCrop, a model developed by the Food and Agriculture Organization of the United Nations, is one of several different models that aid water management related to crop production. AquaCrop has been largely used for evapotranspiration calculation due to its strong equilibrium between robustness and precision (Farahani et al., 2009). AquaCrop is a general model for a large range of agricultural production (herbaceous crops, forage, vegetable, grain, fruit, oil, root, and tuber crops). In general, AquaCrop has been used to simulate crop development, yield production and water-related variables such as evapotranspiration, Water Use Efficiency, and water productivity, while considering different stressed conditions (Greaves and Wang, 2016), such as: the leaf growth and canopy expansion, the stomatal conductance and canopy senescence, the pollination failure and the harvest index (Greaves and Wang, 2016). Different studies around the world have been conducted using AquaCrop, with some examples being: the simulation of Water Footprint of woodies in China (Poppe, 2016), calculation of irrigation technologies for Cotton Water Footprint (Zouidou, 2017), and my own work (Barros et al., 2022).

FAO had as the main goal to build a new model would be simple enough but at the same time adequate and accurate enough to be used by the research community and anyone who would be interested (Steduto et al., 2009), as without the need of complex and sometimes difficult to obtain inputs for the model calculation, AquaCrop could simplify and expand and give the availability for a reliable and simple crop growth model (Vanuytrecht et al., 2014). AquaCrop model can be quite effectively used to model and build a water productivity and management, and it has been receiving many updates since its release in 2009, improving the efficiency in which users can use it (Vanuytrecht et al., 2014).

With these updates that have been occurring to the model, new standardized crops and soils have been added to the examples that the model provides, facilitating in this way as well different researchers, as they can use these files and roughly estimate what would be happening in the field (Panek-Chwastyk et al., 2024). These files utilize some conservative parameters, and because of these parameters it has been possible to utilize them, and sometimes with just some minor adjustments to them, properly estimate yield of the same crop in different parts of the world (Maher et al., 2021).

With the rise in the utilization of the AquaCrop model, more complex researches in different fields like, crop and field management (Alvar-Beltrán et al., 2023), water management (Steduto et al., 2009), effect of climate change on crop yield (Vanuytrecht et al., 2014), have been appearing throughout the years, and sometimes a point based approach, which the AquaCrop model provides (AquaCrop, 2024), would not be sufficient for some cases. For that some tools have been created to ameliorate that issue, for example AquaData, Danube Data Cube (Danube Data Cube, 2025) and AquaGIS (Lorite et al., 2013). These tools use most of the time as a base the external plugin that FAO has developed as well for AquaCrop (AquaCropB, 2024), which is the model but without the user interface to modify the different inputs and parameters needed for the modeling, instead the plugin utilizes some text files (which could be created in the normal AquaCrop software or manually) to provide the necessary inputs (AquaCropB, 2024). The package created during the time of this thesis uses this plugin in an R environment and manages to run the AquaCrop package utilizing raster based inputs, providing an easier alternative to process raster based data with AquaCrop (Barros et al., 2022).

2. OBJECITVES

The main objectives of the work included in this thesis were the following:

1. Development of a methodology for the raster-based spatial application of the AquaCrop model.
2. Application of the developed methodology in an R-based (open-source) environment.
3. Testing and evaluating the resulting R package through 5 study cases.
4. Using the developed package, evaluating the available spatial soil datasets for Hungary, with focus on their potential use for the spatial extension of the Hungarian Drought Monitoring System.

3. LITERATURE REVIEW

3.1. Water resources

Water use per capita is increasing and it has been seen that water issues start to be among the top challenges that global leaders are facing (SIWI, 2016). Domestic, industrial, and agricultural water demands are set to increase and might grow by up to 40% for the next years (US National Intelligence Council, 2013) and with human activities usually having a negative effect on water resources, due to consuming or polluting the existing water resource water scarcity will tend to increase (Hoekstra et al., 2009). Moreover, water scarcity increases especially due to climate change, which alters rainfall patterns and leads to the increase of extreme weather events (SIWI, 2016). This situation may result in low availability of freshwater in many regions of the world due to the different ecological and climate patterns.

The demand for water has been increasing in most sectors, its total consumption can be considered as the total independent water demand of it (Hoekstra et al., 2009). The water demand sources that are mainly present are agriculture, industrial activities, energy production, and human water consumption (UNWWDR, 2003). Economic development and an increase in population lead as well to an increase of water demand, and in addition to that in agriculture, water consumption is determined by irrigation and livestock needs, which depends on the plant's types, the growth, the soil characteristics, and the climate patterns of the agricultural region. Agriculture water demand represents over two-thirds of the global water use (Jason et al., 2009).

Agriculture represents 70% of the total freshwater withdrawals and 11% of world's land use, and therefore presents the highest risk of water scarcity (FAO, 2011). Rain-fed agriculture is the most predominant worldwide, however, evapotranspiration from irrigated land contributes to high water use. With population increase it is expected that the increase in land use for agriculture will increase as well, with that water scarcity may become more recurrent (Jason et al., 2009). So far, an increase from 2.5 to 3 times over time of agricultural production has been seen in the globe, in which 40% came from irrigated areas, this increase in production came from better management but as well from an increase of 12% of areas used for cultivation (FAO, 2008). Agriculture is, at the same time, a cause and a victim of water scarcity, as indeed agricultural production is known as one of the responsible for greenhouse gas emissions (13.5% (IPCC, 2007)) and water depletion (Lovarelli et al., 2016), but is at the same time, one of the biggest victims of water scarcity.

3.2. Crop Water Management Background

Soil infiltration is one of the most important processes when it comes to the environmental and agricultural fields, because it provides the information necessary to determine runoff and recharge at a site (Lowery et al., 2015**)**. Soil properties are heterogeneous and change in both horizontal and vertical directions The spatial heterogeneity of soil affects infiltration while infiltration is further influenced by other factors like land cover, surface slope and climate which governs evapotranspiration (Rasheed et al., 2022). Soils are a critical natural resource in Hungary, their proper mangement is critical in managing climate-related anomalies (Várallyay, 2015). There are several methods to measure infiltration rate like, saturated hydraulic conductivity, cumulative infiltration and other infiltration characteristics of soil with high precision. The most common of these methods is the infiltrometer, which is very useful for measuring infiltration rate at a specific location or point during a particular time frame (Reynolds, 1993). Since infiltration properties vary with time, position and moisture condition, accurate measurements of infiltration rate over the period of a 2 few hours and in a relatively small area is a tedious and time-consuming job requiring extensive labor and resources. In these circumstances, there is a need for continuous observation of soil properties, soil moisture and infiltration processes in micro scale as these processes are complex and of significant importance (Thomas et al., 2020).

These data are important in situations like flood prevention agricultural applications and stormwater management. Given accurate and real-time soil infiltration properties, plant characteristics and soil moisture content would allow for effective irrigation scheduling to provide sufficient water and reduce water loss through runoff (Muñoz-Carpena, 2019). Application of soil moisture sensor based system helps to increase productivity in agriculture (Muñoz-Carpena, 2019) and to obtain design parameters in modeling of stormwater system with soil information increases productivity up to 100% (Clark et al, 2008), while application of ground penetrating radar (GPR) is a possible way to derive information on soil moisture availability (Herceg and Tóth, 2023), its application during growing season and at larger scales is currently very limited. Modern real-time field sensors, including soil moisture sensors, are cheap, accurate and can provide data at intervals of seconds. Previous research has shown that water use is reduced by up to 51% by application of automatic soil moisture sensor-based irrigation as compared to traditional timer-based irrigation (Haley & Dukes, 2007; Clark et al., 2008). The system needs only weekly maintenance once it is set up and verified (Dukes et al, 2003).

There are more straightforward approaches for crop water management, some of these are: utilizing up to date machinery and automated network for controlling water input, striving to diminish the total usage of soil and water, utilize prediction models to monitor changes like drought, flood, climate changes and others (Mandal et al, 2021).

3.3. Soil Physical Properties

Knowledge of soil hydraulic properties is essential for understanding and evaluation of the physical and chemical processes involved in flow of water and transport of dissolved material in a system (Al-Jabri et al., 2002). Reliable results from numerical models of water flow and solute transport are critical for use by any regulatory agency or research project. The accuracy of predictions is often limited by different things, like. the adequacy of hydraulic property estimations (Mertens et al., 2005; Wesseling et al., 2007) These relationships are strongly non-linear and behaves differently for each soil layer. Many analytical equations, which have been incorporated in different models, have been developed to describe these relationships in a simple way (Wesseling and Ritsema, 2009; Rudiyanto et al., 2020; Leij et al., 1997).

3.3.1 Soil phases

Soil is a multiphase and particulate material that usually consists of different mingled solids, water and air. Or more appropriately, soil is a layer on earth's surface that has been weathered and has water and air in the porous spaces and voids between mineral grains, organic materials and rock fragments

(Wesseling and Ritsema, 2009; Jopffe, 1949). Soil is composed of primary and secondary minerals, primary minerals are soil materials like the parent materials they are formed of; secondary minerals are stable mineral forms which are obtained by weathering of primary minerals (Jopffe, 1949).

Mineral particles present in soil can be mainly categorized as sand, silt or clay. Sand has the largest particles size, with large pore spaces around it causing higher porosity and improved aeration (Wesseling and Ritsema, 2009). Silt has medium particles and clay has the smallest particles of the three. Mostly due to the particle size hydraulic conductivity is very high in sand and the lowest for clay (Svensson et al., 2022). Size of sand, silt and clay are 0.05 to 2 mm, 0.002 to 0.05 mm and less than 0.002 mm respectively (Moreno-Maroto et al., 2022).

Texture of soil and its properties depend upon its percentage of sand, silt and clay, demonstrated by the United States Department of Agriculture (USDA) soil classification textural triangle (Moreno-Maroto et al., 2022), show on Figure 1. Organic matter takes up to 5% of soil volume and has high water holding capacity helping plant growth, and in turn affecting soil moisture in a way that maintains different levels of soil moisture (Idowu et al., 2020). The composition percentage of different parameters in an average soil can be defined as, average water content in soil is around 25%, being vital for plant growth and biological organisms present in soil, mineral materials occupy 45% of soil volume while air occupies around 25% of soil volume and provides oxygen for roots and microbial respiration for plant growth (Idowu et al., 2020)

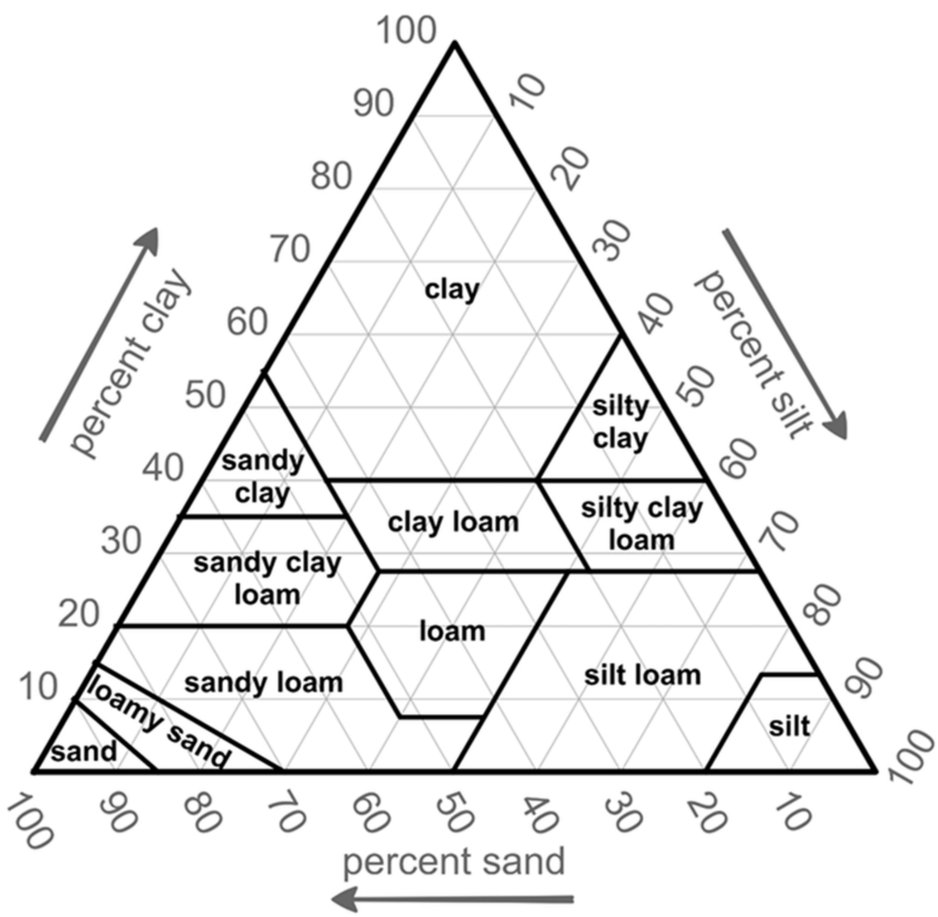


Figure 1 – Soil texture characterization USDA (Groenendyk et al., 2015)

3.3.2. Soil Moisture

Soil moisture content is very important in defining different soil parameters, but most importantly hydraulic conductivity and infiltration characteristics, with soil composition having a profound influence on moisture bearing capacity retrospectively (Srivastava et al., 2019). Clay has higher surface area than silt and sand, resulting in greater water holding capacity and higher water holding capacity inversely influences soil infiltration (Srivastava et al., 2019), this makes knowing the percentage of clay especially important for understanding infiltration and water-holding capacities in different soils (Almendro-Candel et al., 2018). Soil moisture is responsible for change in physical, chemical and biological properties of soils (Edwards and Cresser, 1992). Deák et al., 2023 have found in their study that soil physical parameters (particularly porosity and bulk density have provided the best correlation with soil moisture dynamics. However, they also indicated that geomorphological parameters were the most dominant co-variates, independent of season. Ujj et al., 2019 has also found that topography was a significant factor in soil moisture dynamics.

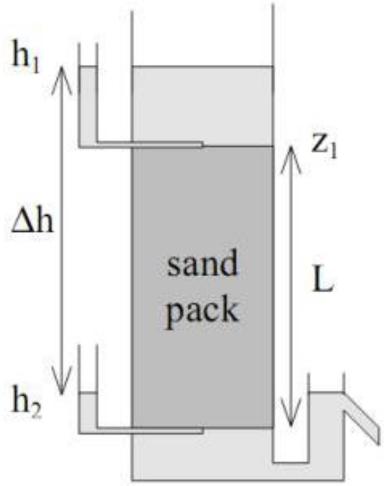
Soil moisture content or water content can simply be defined as the amount or quantity of water the soil or soil subsurface contains with volumetric units (cm^3/cm^{-3}) and gravimetric units (represented as volume of water/ volume of oven dried soil) (Rahmati et al., 2024). Even though the volume of moisture in soil is insignificant when compared to large volumes of water within other components in the hydrologic cycle, it has a significant impact on many hydrological, biogeochemical, biological processes and as well the runoff from precipitation that would go to a nearby water body (Li et al., 2016).

Replenishment of soil moisture happens from precipitation, irrigation, overland and subsurface flow of water and capillary rise from the water table (Li et al., 2016). Percolation is an event for soil water loss to lower unsaturated layers when a precipitation event is higher than infiltration rate, when that happens an overland water flow is expected, which does not replenish the soil water content (Phillips, 2017). In another way of putting infiltration and percolation, it can be said that infiltration is water entering soil surface, increasing soil moisture content and percolation involves water passing through soil layer into ground water, decreasing soil water content (Phillips, 2017).

3.3.3. Hydraulic Conductivity

Hydraulic conductivity (Ksat) is the measure of ease for water to pass through a medium or soil, hydraulic conductivity of a soil is considered the most important soil property, which affects the design of water-table management systems (Doty et. al, 1986), describing the water movement through the soil profile (Dorsey et al., 1990) and important in different infiltration models. Hydraulic conductivity is further understood as the ability of a porous medium to allow water to flow through it due to pressure gradient (Zhang, 2002).

Darcy’s law can explain how hydraulic conductivity works in the soil. According to Darcy’s law (Darcy, 1856), $q = KA(h_1 - h_2)/L$ (Figure 2), the volumetric rate can be calculated with the equation seen on Figure 2.



$$q = KA\frac{(h_1 - h_2)}{L}$$

q: volumetric rate [m³/s]
K: hydraulic conductivity [m/s]
A: Cross-sectional area of sand pack [m²]
h: piezometric head [m]
L: length of sand pack [m]

Figure 2 – Darcy's law diagram (Darcy, 1856)

This equation is known as Darcy's equation and the value $(h_1\text{-}h_2)/L$ represents hydraulic gradient(s), which is the difference of head $(h_1\text{-}h_2)$ over a length of L as shown in figure 2.

Hydraulic conductivity value of a saturated soil depends mainly upon size, shape and distribution of pores and is also affected by soil temperature, viscosity and density of water (Oosterbaan and Nijland, 1994) and thereafter soil texture affects the hydraulic conductivity. Figure 3 shows different relationships between soil classification and different processes in the soil.

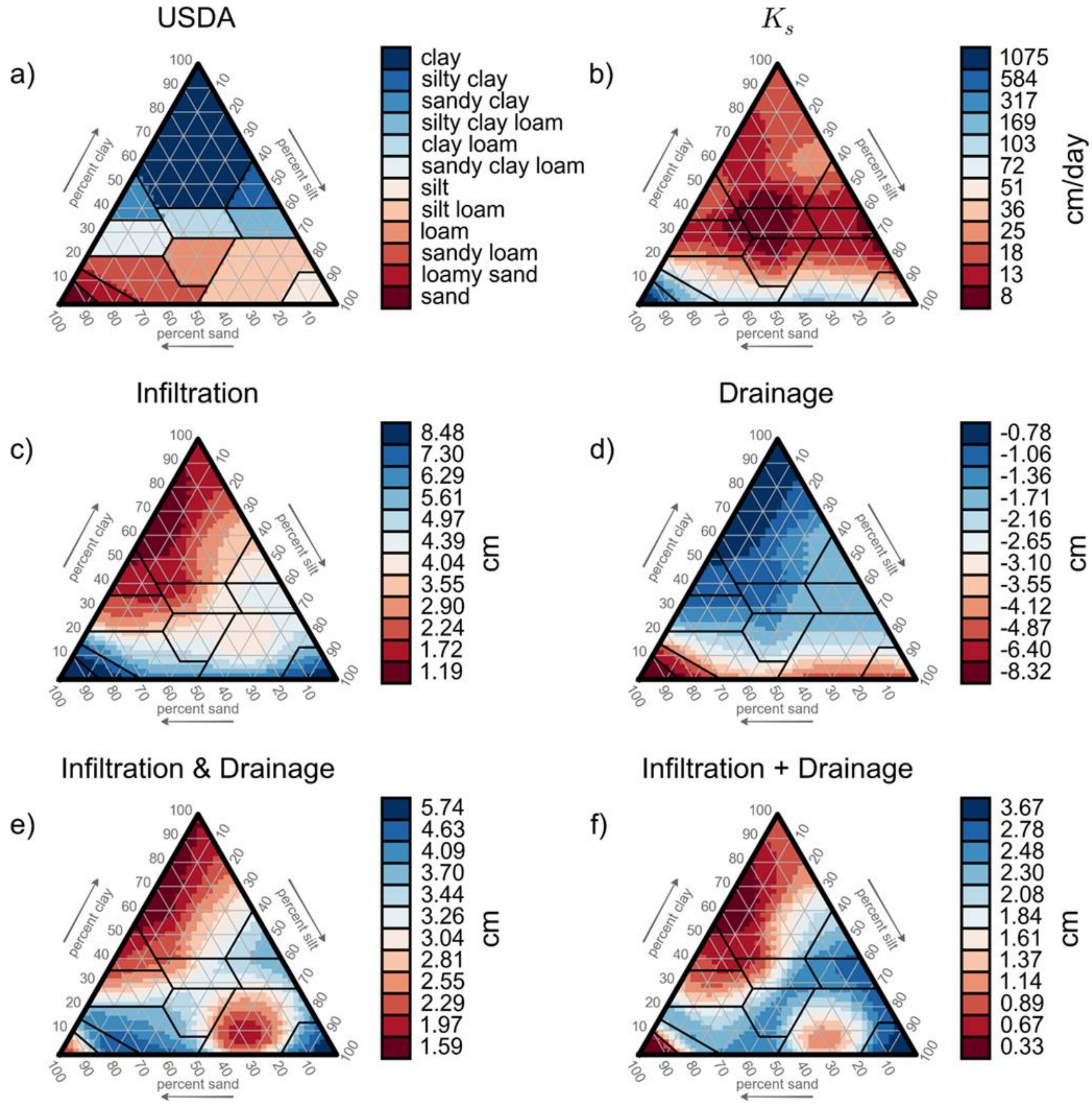


Figure 3 – Soil classification and soil processes (Groenendyk et al., 105)

Hydraulic conductivity is a function of soil moisture conditions and soil suction (Dorsey et al., 1990), if all pores of soil are filled with water, then soil is said to be saturated and the entire pore space of soil will be able to conduct water. The soil water flow is mainly under influence of gravity in saturated soil and pressure gradient depending upon the amount of soil moisture in unsaturated soil, meaning that the water would flow from a more saturated to a less saturated section of the soil (Oosterbaan and Nijland, 1994), with the soil suction becoming more important as soil moisture content decreases (Dorsey et al., 1990).

Knowing saturated hydraulic conductivity is important as it is useful in drainage design and in computation of velocity with which water can move towards and into drain lines below the water table

(Amoozegar and Wilson, 2015). Hydraulic conductivity is important for infiltration rate as it mainly determines how easily water can flow through the soil and it is a measure of soil's resistance to flow (Turner et al, 2018), as saturated hydraulic conductivity is used as a parameter in many infiltration equations as it is easier to determine than the unsaturated hydraulic conductivity.

3.3.4. Soil Infiltration

Soil infiltration is defined as the ability of soil to absorb water. Cumulative or total infiltration can be measured in terms of depth of water infiltrated into and through the soil layers (Cai et al., 2023) and it is an important parameter as it can be used to determine runoff value from watersheds, which runoff being a really important parameter for environmental reasons (Rasheed et al., 2022). The soil infiltration rate is the speed at which water passes through the soil per unit time and the difference between hydraulic conductivity and infiltration rate is that hydraulic conductivity is an intrinsic soil property while the infiltration rate depends mainly upon potential difference, hydraulic conductivity, diffusivity, porosity, initial moisture content and water holding capacity of soil (Amoozegar and Wilson, 2015).

Arable soil in good condition has a stable structure with continuous pores, resulting in good infiltration of water into and throughout the soil, reinforcing the necessity of proper techniques in the soil, as low infiltration rate is observed due to soil sealing and soil crusting (Turner et al., 2018). Besides that, infiltration is caused by gravitational force and capillary action where gravitational force acts in the direction of gravity while capillary action is pulling movement of water through very small pores and is caused by surface tension force of water (Amoozegar and Wilson, 2015) and capillary action could be in the same or opposite direction of gravitational force.

The effects of different infiltration rates are notable in the field, a low infiltration rate leads to reduced base flow and increased storm flow (Walsh et al., 2012), surface soil erosion (Tsihrintzis and Hamid, 1997), not a proper level of moisture for crop production and runoff of surface applied fertilizers and pesticides on sloping landscapes. Substances carried by runoff can pollute water bodies and sources (Tsihrintzis and Hamid, 1997), which can result in different and unwanted chemicals and materials entering the water system, this being one of the main sources of water pollution throughout the U.S (EPA). Without regulation or water quality controls, runoff can lead to harmful effects on the environment and human health (Tsihrintzis and Hamid, 1997). Therefore, infiltration is one of the prime factors in runoff management. Additionally, with a high infiltration rate, fertilizer and pesticide leaching into groundwater might happen and necessitating proper chemical management to protect groundwater (Tsihrintzis and Hamid, 1997).

When the water application rate is lower than the soil's infiltrability, water completely infiltrates through soil and when water application rate is higher than the soil's infiltrability then ponding happens over soil surface (Williams et al., 1998), which means that infiltration is dependent on the water application rate. At the beginning of the infiltration process, infiltration rate is very high and decreases rapidly and eventually attains a stable rate almost equal to saturated hydraulic conductivity of soil (Turner et al., 2018). For dried soil, infiltration rate takes some time to attain stable value and for wet soil, a stable infiltration rate will be more quickly attained. Other factors that can affect infiltration rate are, soil texture, compaction, surface crust, aggregation, water content, hydraulic conductivity, organic matter, pore types and frozen surface (Thomas et al., 2020; Santos et al., 2018).

There are quite a few infiltration models describing how the infiltration process happens, there are three types for these models, physical based models, approximate models and empirical models (Thomas et al., 2020). Physical based models approaching Richard's equation (Maskey, 2022) describes water flow in soils as hydraulic conductivity and the soil water pressure as functions of soil water content, for specified boundary conditions. Physical based models are highly dependent on soil properties like saturated hydraulic conductivity and soil moisture gradient. Empirical models, as their parameters are calibrated differently for different conditions as these parameters are determined by curve fitting or other means, like Horton and Holtan models (Thomas et al., 2020) may give better results than the physical ones, but that is dependent on their input data.

3.4. Water footprint concept

The concept of water footprint relates to the virtual water concept that Allan (1998) has introduced (WWF, 2009). The virtual water illustrates the total water consumed for a good or services production as it refers to the water embedded in the global water trade. Virtual water is the required water volume for any production (Hoekstra et al., 2011). The calculation for virtual water considers all the water sources, directly or indirectly, used to produce any good. The concept was applied to quantify the water content from the surface, groundwater, and water from rainfall. The virtual concept has mainly been used to influence decisions on water use in consumption, production, and trade of products (Frontier economics, 2008).

Hoekstra came with the water footprint concept, in 2002 (Hoekstra et al., 2011), which is closely related to the virtual water concept. Water footprint can be defined as an indicator of water use (direct and indirect) of a producer or consumer, it is the total freshwater volume consumed for goods and services production which are consumed by any entity (individual, community, business). Water footprint is a tool to evaluate the agricultural production, environmental impacts, and water resources relationship to increase water use efficiency, water sustainability and water management (Mekonnen and Hoekstra, 2011; Lovarelli et al., 2016). Moreover, it is a water management tool, which allows the comparison of water consumption, pollution, production, and water availability in a determined area. For example Jolánkai et al. (2021) have utilized the concept to assess the water footprint of protein formation of crop species.

Water footprint has three components: blue, green, and grey. The blue water footprint represents the blue water resources consumption which means the loss of water from the ground surface or surface of a water body in a catchment area, referring to the groundwater or surface water consumption and more specifically for the crop. it represents the evaporated water during crop development from groundwater and surface water (Hoekstra et al., 2011). Green water footprint represents the green water resources consumption which indicates the consumption of rainwater. It is the evaporated water through crop development from rainfall (soil moisture). The green water footprint measures the rainwater volume used throughout the production. It is mainly available for agricultural and forestry products which refers to the incorporated water and evapotranspiration water in wood or harvested crops (Hoekstra et al., 2009). Finally, the grey water footprint represents the water pollution which represents the required freshwater volume to assimilate the pollutants load entering freshwater bodies, after consideration of the water quality standards (Hoekstra et al., 2011), figure 4 shows how the different types of water footprint are separated.

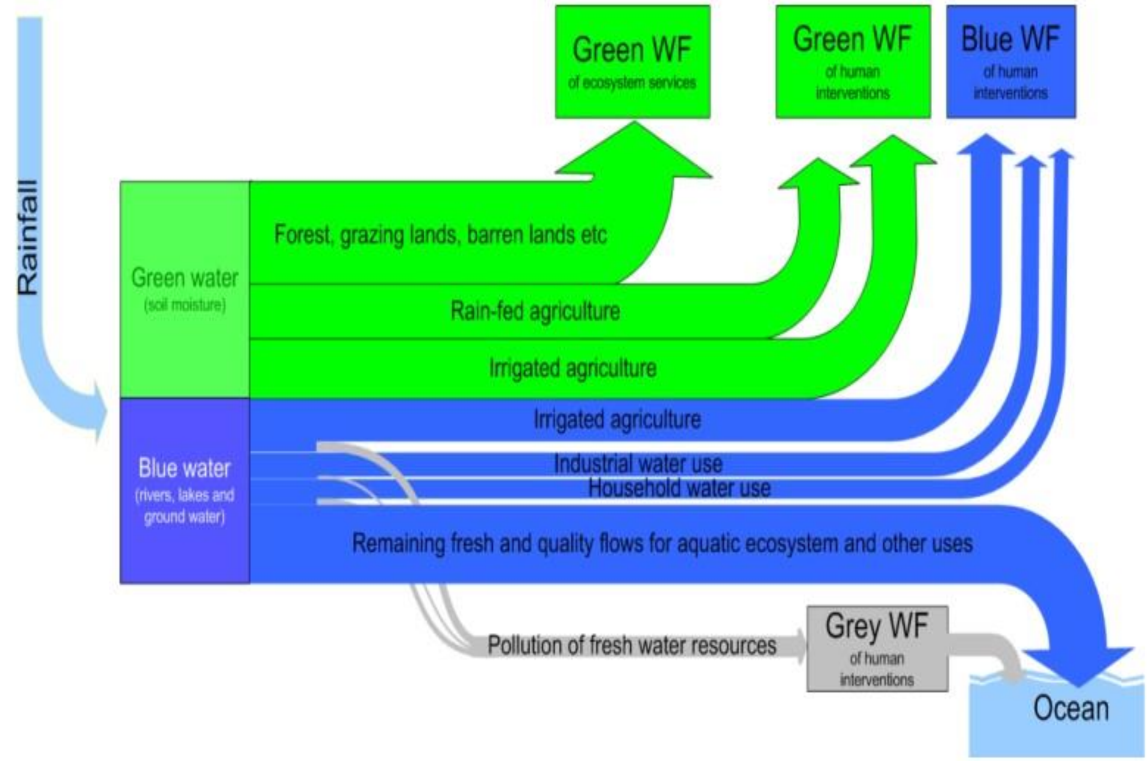


Figure 4 - The three types of water footprint (Source: Chapagain and Tickner, 2012)

3.5. The AquaCrop model

AquaCrop model is used for different types of agricultural production (such as herbaceous crops, forage, vegetable, grain, fruit, oil, root and tuber crops), it is a model that tries to simplify the crop simulation model calculation (Steduto et al., 2009). Crop response to water deficit has always been a complex process to understand, so AquaCrop aligns along with the need of water productivity calculation improvement. This and other changes like, reviewing on how to treat different types of crops, and different scenarios that they can appear, as the model was designed to simulate crop growth in different scenarios (Steduto et al., 2009).

The AquaCrop model aims to examine the crop yield change especially under different environmentally stressed conditions (Greaves and Wang, 2016). The model intends to simulate the yield and crop growth using the water-driven growth model considering the influence of soil moisture variation trough time. AquaCrop is a simpler model when compared to other models, but it can be described as having a good equilibrium between precision and robustness (Farahani et al.,2009), as it simulates the full development of a crop through the simulation period and calculates total biomass utilizing the amount of transpired water and yield (Studeto et al., 2012).

The thing that separates this model to others is that it calculates separately the soil evaporation and the crop transpiration before the actual evapotranspiration, this was done to avoid the confusion effect of the nonproductive consumption water use, also, it works with the green Canopy Cover as an alternative of the leaf area index. The calculation of transpiration for stress-free condition requires the crop coefficient to be set with the canopy cover and base evapotranspiration whereas for the soil evaporation, the soil evaporation coefficient is required. Besides that, AquaCrop simulates the daily water balance calculation, which it considers the incoming and outgoing fluxes, and therefore simulates the root zone water changes (Raes, 2017). AquaCrop model considers four main water stress coefficients in its simulation, which are leaf growth and canopy expansion, stomatal conductance and canopy senescence, pollination failure and harvest index being the last one (Steduto et al., 2009).

The atmosphere system parameters are represented by five different weather input variables, them being, minimum and maximum air temperatures, rainfall, evaporative demand of the atmosphere (ET_0) and the mean annual CO_2. On the other hand, the crop system introduces five components, which are the phenology, green canopy cover, the rooting depth, the biomass production, and the harvestable yield (Steduto et al., 2009). All of these systems together take in consideration the rooting depth together with the root-water extraction, with in the end a water balance is taken in consideration, which includes infiltration, runoff, drainage, deep percolation, crop uptake, capillary rise, evaporation and transpiration (Steduto et al., 2009).

A visualization of the AquaCrop simulation scheme can be seen at figure 5 bellow.

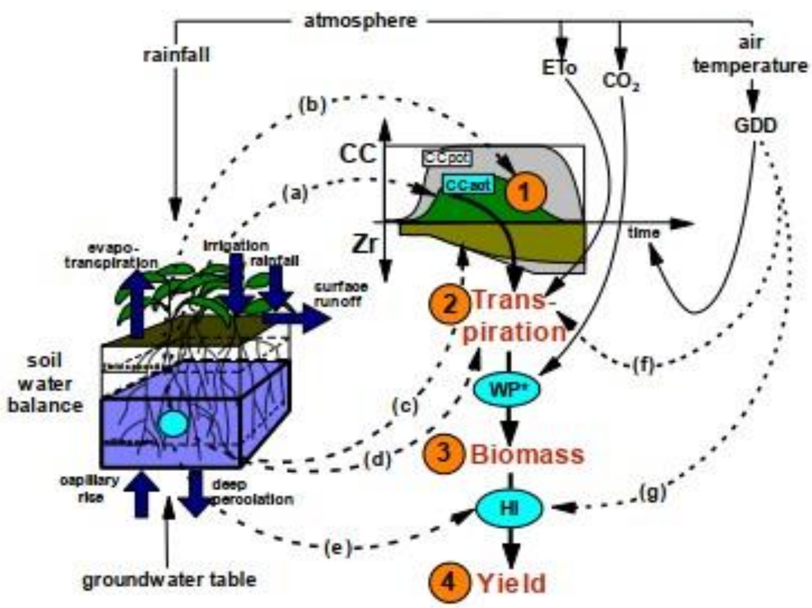


Figure 5 - AquaCrop calculation scheme (Raes, 2017)

For the legends, CC is green canopy cover; Zr is rooting depth; ETo is reference evapotranspiration; WP* is normalized biomass water productivity; HI is harvest index; and GDD are growing degree days. For how the water stress affects in the different processes: (a) slows canopy expansion, (b) accelerates canopy senescence, (c) decreases root deepening but only if severe, (d) reduces stomatal opening and transpiration, and (e) affects harvest index. Cold temperature stress (f) reduces crop transpiration. Hot or cold temperature stress (g) inhibits pollination and reduces HI (Raes, 2017).

As seen in figure 5, there are four main parts for the calculation scheme of AquaCrop, number 1 is the simulation of the crop development based on the canopy cover growth (phases are: from transplanting to recovered transplant, transplant to maximum rooting depth, transplanting to senescence, transplanting to maturity and transplanting to start of yield formation) (Raes et al., 2009), number 2 is the simulation of crop transpiration which follows the equation bellow.

$$Tr = Ks\left(Kc_{Tr,x}CC *\right)ETo \tag{1}$$

Equation 1 – Daily transpiration calculation (Raes et al., 2009)

$Tr \rightarrow Daily\ transpiration\ ammount$

$Ks \rightarrow Stress\ coefficient$

$Kc_{Tr,x}CC \rightarrow Crop\ coefficient$

$Eto \rightarrow Atmosphere\ evapotranspiration$

Number 3 refers to the simulation of above ground biomass production, which is calculated following the equation bellow.

$$B = Ks_b WP \sum \frac{Tr}{ETo} \tag{2}$$

Equation 2 – Daily above ground biomass equation (Vanuytrecht et al., 2014)

$Tr \rightarrow Daily\ transpiration\ ammount$

$B \rightarrow Biomass\ production$

$WP \rightarrow Wilting\ point$

For the last phase of calculation, the aim is to get the total final crop yield for the simulation, which can be seen in the equation bellow.

$$Y = f_{HI} HI_o B \tag{3}$$

Equation 3 – Daily yield calculation equation (Vanuytrecht et al., 2014)

$Y \rightarrow Total\ daily\ yield$

$f_{HI} \rightarrow Water\ stress$

$HI_o \rightarrow Harvest\ index$

Hungarian examples of utilizing the AquaCrop model include its application for tomato (Takács et al., 2021; Takács et al., 2022) and for vine production (Bujdosó & Waltner, 2017).

3.5.1. Water Balance Calculation

As mentioned before the AquaCrop model design has taken in consideration the continuous relations between the soil and atmosphere, figure 6 shows this relation and how every different parameter relationship leads to the plant yield result in the end.

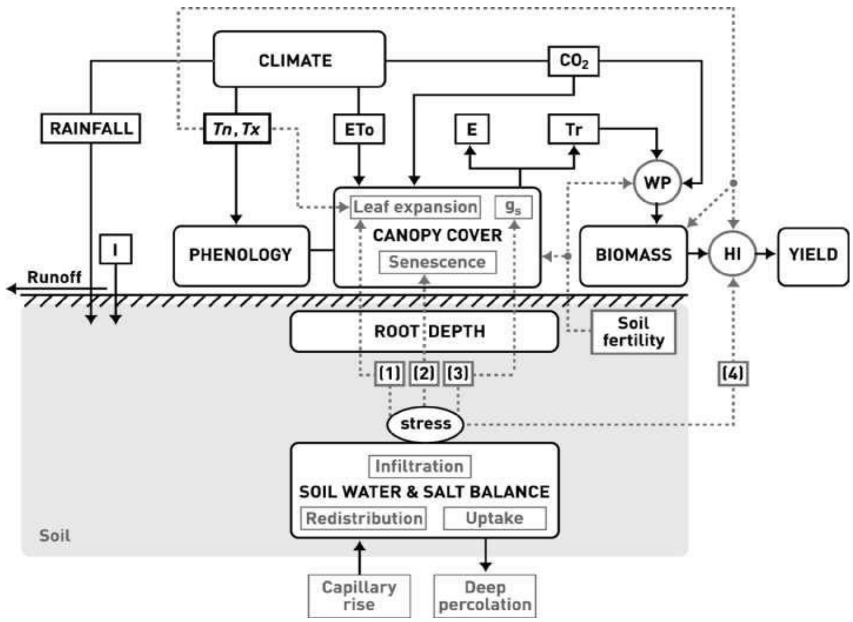


Figure 6 - AquaCrop soil-plant-atmosphere continuun relations and the different parameters considered in it (Raes et al., 2018)

The root zone is taken as a reservoir for the water in the system, and the amount stored is simulated by the calculation of the water fluxes (outgoing and incoming) and its boundaries. The root zone water depletion determines the water stress degree, which affects how the whole system will behave in relation to the available water (parameter such as, green canopy expansion, canopy senescence, stomatal conductance, transpiration, decline of the root system, and harvest index). The simulation of the model always starts with simulating drainage of the soil profile, after it the surface runoff is taken into consideration as well as the water that infiltrates into the soil profile and goes upward by capillary rise. From there, evaporation and transpiration represented by the water loss is calculated. For every subroutine, AquaCrop updates the soil water content at the end of the simulated time and for each point (Raes et al., 2018). Figure 7 shows these relations for the water in the root zone.

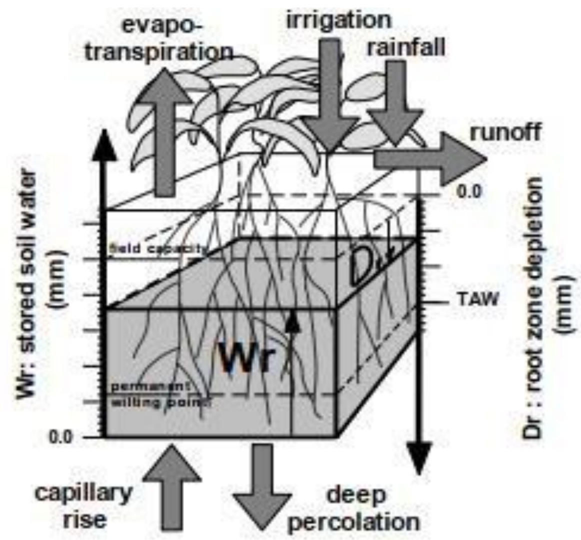


Figure 7 - Water fluxes in the root zone (Raes et al., 2018)

When taking in consideration the water balance simulation for the AquaCrop model, there are different subroutines which were mentioned before, them being, drainage, runoff, infiltration, capillary rise, soil evaporation and crop transpiration (Raes et al., 2018).

For AquaCrop, the drainage simulation is done while utilizing the drainage function (equation 4). This equation illustrates the total water lost between field capacity and saturation by free drainage.

$$\frac{\Delta\theta_i}{\Delta t} = \tau(\theta_{sat} - \theta_{FC})\frac{e^{\theta_i - \theta_{FC}} - 1}{e^{\theta_{sat-FC}} - 1} \quad (4)$$

Equation 4 – Drainage function (Raes et al., 2018)

Where:

$\frac{\Delta\theta_i}{\Delta t} \rightarrow decrease\ in\ soil\ water\ content\ at\ a\ depth\ of\ i\ during\ a\ time\ step\ t$

$\tau \rightarrow drainage\ characteristics$

$\theta_i \rightarrow actual\ water\ soil\ content\ at\ depth\ i$

$\theta_{sat} \rightarrow soil\ water\ content\ at\ saturation$

$\theta_{FC} \rightarrow soil\ water\ content\ at\ field\ capacity$

$\Delta t \rightarrow time\ step$

The decrease in soil water content per day is to be assumed as constant throughout a drainage profile if the soil is equally wet. For non-equally wet soil, the calculation considers the drainage ability of each compartment of the soil. When the soil water content is smaller or equal to its field capacity, the drainage ability is null and then the total drainage amount is the amount of cumulative drainage per compartment (Raes et al., 2018).

The amount of rainfall lost by runoff is calculated in AquaCrop utylizing the curve number, which has been based on USDA classification, using antecedent moisture class (Rallison, 1980). The curve number value is corrected for the simulated wetness of the topsoil layer considering dryness and wetness of it. As mentioned before the saturated hydraulic conductivity of the topsoil layer will limit the infiltration rate and because of that the excess water will be lost as runoff. The equations that simulate the runoff subroutine can be seen bellow.

$$RO = \frac{[P - I_a]^2}{P + S - I_a} \tag{5}$$

$$S = 254\left(\frac{100}{CN} - 1\right) \tag{6}$$

Equations 5 and 6 – Runoff calculation subroutine (Raes et al., 2018)

Where:

$RO \rightarrow ammount\ of\ water\ lost\ by\ runoff$

$P \rightarrow rainfall\ ammount$

$I_a \rightarrow ammount\ of\ water\ that\ can\ infiltrate\ before\ runoff\ starts$

$S \rightarrow potential\ maximum\ soil\ water\ retention$

$CN \rightarrow curve\ number$

After the runoff amount is subtracted from the amount of water input, what is left is the infiltration amount, this infiltrated water in the soil profile is stored to the consecutive compartment from top do lower soil layers, never exceeding the water content threshold (Raes et al., 2018). As this subroutine integrates wetness at its initial point, the amount of infiltrated water per time stage, the infiltration rate and the drainage characteristics of the soil layers this can mimic what happens in the soil (Raes et al., 2018).

For the capillarity rise subroutine calculation, Darcy's equation is used to describe the upward flow from the shallow groundwater table to topsoil, and it is estimated by taking in consideration the soil type and its hydraulic characteristics (Raes et al., 2018). Equation 4 shows how the capillarity rise is simulated.

$$CR = exp\left(\frac{ln(z) - b}{a}\right) \tag{7}$$

Equation 7 – Darcy's equation for calculating capillarity rise (Raes et al., 2018).

Where:

$CR \rightarrow capilarity\ rise$

$z \rightarrow depth\ of\ the\ water\ table\ bellow\ the\ soil\ surface$

$a \rightarrow specific\ parameters\ for\ soil\ and\ its\ hydraulic\ characteristics$

$b \rightarrow specific\ parameters\ for\ soil\ and\ its\ hydraulic\ characteristics$

The calculation of capillarity rise begins from the bottom compartments and moves to the upward layers until the top compartment. In each compartment, water is stored inside until the soil water content is equal to soil water content at Field capacity or all the capillarity rise has been stored (Raes et al., 2018). This being the last subroutine for water balance in the simulation, besides this soil evaporation and crop transpiration are considered as well.

For the soil evapotranspiration calculation, AquaCrop first takes into consideration ET_0, which represents the evapotranspiration rate from a grass reference surface and with that soil evaporation is simulated utilizing the equation 5 and in figure 8 how the calculation scheme works with all the different inputs (Raes et al., 2018).

$$E = (KrKe)ET_0 \tag{8}$$

Equation 8 – Soil evaporation calculation (Raes et al., 2018)

Where:

$E \rightarrow Soil\ evaporation$

$Ke \rightarrow Soil\ evaporation\ coefficient$

$Kr \rightarrow evaporation\ reduction\ coefficient$

$ET_0 \rightarrow Evapotranspiration\ rate\ from\ grass\ surface\ reference$

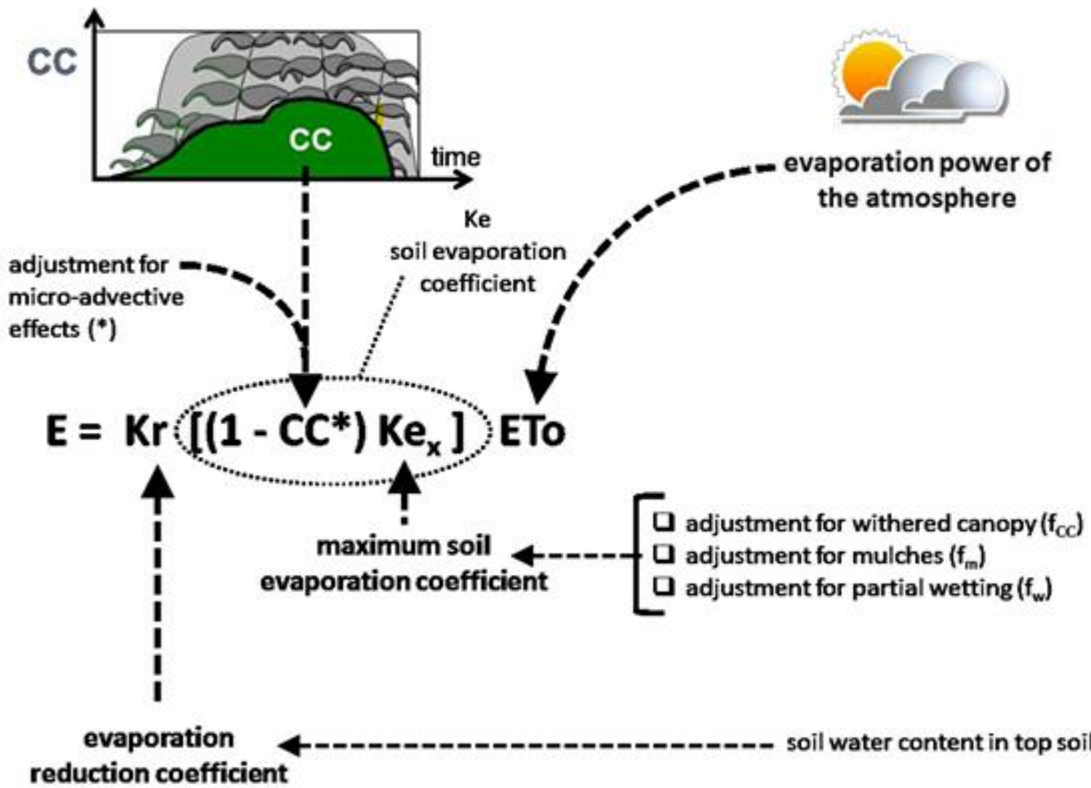


Figure 8 – Calculation scheme for evaporation in AquaCrop (Raes et al., 2018).

The evaporation reduction coefficient is a coefficient related to the soil water insufficiency to answer the atmosphere evaporative demand. It considers the soil water content in the topsoil. The soil evaporation coefficient and the increase of canopy cover are proportional and during the first stage of evaporation called the energy limiting stage, the water is evaporated from the thin soil surface layer which is the soil directly in contact with the atmosphere. For the second stage when all the water is evaporated from the top soil, the water from the bellow departments begin to flow upward to the surface. Another important parameter is the readily evaporable water, which is the maximum water removed from the soil surface (Raes et al., 2018).

3.6. Hydrus model

Hydrus was created as a software package to simulate water, heat and movement of solutes in a one, two and three dimensional media (Simůnek & Šejna, 2022). The Hydrus model resolves the Richards equation for unsaturated-saturated water and heat flown in a porous media. The heat flown transport considers the conduction and convection movement in the system and for the solvent, it considers a dual-porosity system and when taking into account a surface with a plant, the root zone uptake is taken into consideration as well (Simůnek & Šejna, 2022). Hydrus 1D does include as well different modules, with one of its most important is one to simulate carbon dioxide production and ion movements through the solute (Er-Raki et. al, 2021). There are several studies which utilizes the model as a main methodology, like the studies of: Er-Raki et. al, 2021, Yu et, al. 2022, Ventrella et, al. 2019.

4. MATERIALS AND METHODS

4.1. SpatialAquaCrop

SpatialAquaCrop (SpatialAquaCrop, 2022) is the name that was given for the used R based methodology and package that was the main tool for the research of the different study cases in this doctoral thesis. This methodology has been designed to be a user-friendly method in R to read spatial datasets and utilize the AquaCrop plug-in to run the AquaCrop model and then output the results as raster files. In its current version of its script, it can read TIF files, and output the results as a TIF file. The output can be any of the different outputs which the AquaCrop model can give.

SpatialAquaCrop package has different functions which provides an easy way to set up all the necessary data input for running the AquaCrop model in a spatial manner, besides this it has an optional function which can calculate the green water footprint for the whole simulation period.

The primary approach of the package is to run the external AquaCrop plugin software in a way that it will run the AquaCrop model in the specified parameters for each of the points/pixels of the study area, which is represented by a raster files. As mentioned, the package runs the AquaCrop model for each of the different pixel cells and saves the output of each one to be put together in the end again in a raster format or as a table. The AquaCrop plugin utilizes text files to storage all the necessary input data and output data as well, so one of the main functions of the package is to be able to properly input and extract all the information to/from the necessary text files. One important point to take into consideration is that the AquaCrop model is not built in to consider affects from lateral movement from different pixels, which might influence spatial patterns that might have been there, due to mainly topography effects. Because of that even though the package is built in to create spatial datasets, in the future topography effects and lateral movements will have to take into account to more precisely assert the modeled results.

AquaCrop model can be run with many different inputs, depending on what is necessary to be focused or on how much information there is for the run (Raes et al, 2017). These inputs are climate data (precipitation, maximum and minimum temperature, reference evapotranspiration and atmospheric CO2 concentration), crop data, field management, irrigation, groundwater table, initial conditions of the model (if present), soil parameters and the off-season conditions (if existent) (Raes et al, 2018). Even though all these parameters can be used to alter and enhance how the model will be run, not all of them need to be present for the modeling to be performed. A modeling run with minimal parameters needed for it are one that uses only: the climate data, crop data and soil parameters data.

All the parameters that will be used as inputs for the modeling run have to be formatted in a specific formatting in which AquaCrop plugin can read them. SpatialAquaCrop makes sure that all the necessary text files are in the proper formatting, or if the user would want, it is possible to create the text files utilizing the AquaCrop software and SpatialAquaCrop can read the information in those files as well, having the ability to choose where to prepare the input files is a good option, as users who have more experience with the AquaCrop model might prefer to prepare all files with the AquaCrop software. Below is an example of a text file for the base evapotranspiration and how its formatting looks like, which is similar for all the climate text files (figure 9).

```
 input  : monthly data from CARPATCLIM
  1  : Daily records (1=daily, 2=10-daily and 3=monthly data)
  1     : First day of record (1, 11 or 21 for 10-day or 1 for months)
  1     : First month of record
 2020   : First year of record (1901 if not linked to a specific year)

  Average ETo (mm/day)
=======================
     0.6
     0.7
     0.3
     0.5
     0.5
     0.6
     0.6
     0.5
     0.7
     0.8
     0.8
     0.4
     0.2
     0.3
     0.3
     0.3
     0.2
     0.2
     0.2
     0.4
     0.4
     0.6
     0.7
     0.7
     0.4
     0.6
```

Figure 9 – Evapotranspiration input text file

As of this version of the package there are three scripts which represent the three main functions that aim to gather all the necessary information for AquaCrop plug-in to run and produce the different outputs, which will later be presented in a raster format. Besides being a simpler approach for running the AquaCrop model for spatial data, the package aims to be user friendly as well, following on one of the aims of the AquaCrop model (Raes et al, 2018), which is to simplify the process of crop modeling. This package has been developed in an R environment. It is beneficial if the user has a bit of programing knowledge in R but not necessary, as the package tries to guide any user in an easy/understandable way. An overview of what each of the three functions represent can be seen in Table 1.

The Initial function is called 'Initial_AQC ()', it aims to give the user options on how the run will be conducted, which in this case means, which parameters will be used from the ones that AquaCrop can accept. This is done by utilizing the package "svDialogs" (Grosjean, 2022), which gives the user different questions in which depending on the answer the function will know how to proceed and which parameters to take into consideration for the modeling run. In this part the function gives the option as well that if the user would like to use files created from the AquaCrop software, now would be the time to create them and put them into the indicated folder, which it is mentioned during this initial function. At the end of this initial function an external table is created in which the user will have to manually fill in the different information presented there, this will guide how and where the next function will obtain the data necessary for the run. Besides this table, several others might be created as well if the user would like to consider groundwater, field management, irrigation or initial conditions.

After the table has been filled the next function can be initiated, which is called “Control_AQC ()”. This second function’s main objective is to create some of the several unique text files in which the main function, the third one, will be used to run the model. In the beginning this function checks of the model will consider groundwater, field management, irrigation or initial conditions and let the user know that with messages as well, so that the user has a better grasp if the model is considering the right selected parameters. Next a blank crop file will be created in case the user would like to manually fill it, or if it is set that an already filled crop file will be used, a message will be shown mentioning it. The final of these initial files is the CO_2 concentration file, which the standard file that AquaCrop provides has been used.

The next important step of this function is the creation of the project file, which acts as main information holder for the AquaCrop plugin to know the paths of the unique text files, so it can read all the different data inputs necessary for the model calculation. Besides this this file has some standard values that the model will consider, like: Beginning and end date of the simulation run, starting depth of root zone expansion curve, thickness of top soil in which soil water depletion has to be determined and others. Standard values, given by AquaCrop, software for these parameters were used, these values are provided in examples in AquaCrop. One important aspect of this file is that AquaCrop has a special way to read dates in these text files, so for that a small conversion function was created for that purpose, which is present inside the function “Control_AQC ()”, this date conversion function can be seen bellow.

```
Date_count <- function (Year, month, Day){
  Y_1901 <- if(as.numeric(Year) < 1901){ print (" Year is in the wrong place or not in the range
of 1901 to 2099 ")
  } else if(as.numeric(Year)> 2099){ print (" Year is in the wrong place or not in the range of
1901 to 2099 ")
  }else {Y_1901 <- as.numeric(Year)-1901}
  Yx365 <- Y_1901*365.25
  Ymonth <-  if (as.numeric(month) > 12) { print (" months are from 01 until 12 only")}
  else if (as.numeric(month)== 01){Ymonth <- Yx365+0
  }else if (as.numeric(month)==02){Ymonth <- Yx365+31
  }else if (as.numeric(month)== 03){Ymonth <- Yx365+59.25
  }else if (as.numeric(month)== 04){Ymonth <- Yx365+90.25
  }else if (as.numeric(month)== 05){Ymonth <- Yx365+120.25
  }else if (as.numeric(month)== 06){Ymonth <- Yx365+151.25
  }else if (as.numeric(month)== 07){Ymonth <- Yx365+181.25
  }else if (as.numeric(month)==08){Ymonth <- Yx365 + 212.25
  }else if (as.numeric(month)== 09){Ymonth <- Yx365+243.25
  }else if (as.numeric(month)== 10){Ymonth <- Yx365+273.25
  }else if (as.numeric(month)== 11){Ymonth <- Yx365+304.25
  }else {Ymonth <- Yx365+334.25}
  YmonthD <- if (as.numeric(Day)>31){print (" Days are wrong, it should be from 01 until 31")}
```

```
else {YmonthD <- as.numeric(Ymonth)+as.numeric(Day)
Yinteger <- as.integer(YmonthD)
return (Yinteger) }}
```

The final part of the "Control_AQC ()" function is to extract all the input data that are in raster format and export it to different CSV files that will be read in the next function for the modeling calculation. To read and extract the information from the raster files some different packages were used for than, being then sp (Pebesma et al., 2005) and raster (Hijmans, 2024) The goal is to run the model simulation for each of the pixels in order, store the different outputs and in the end put them back into a raster format and a table format as a CSV file for easier access of the result values. The way all the information from the raster files can be extracted and exported into a proper and accurate format is to vectorize the different raster, making larger data sets lighter and easier to read. One detail which was only taken into consideration after analyzing big datasets (for example soil parameters for the whole country of Hungary) is that the CSV table format that has been used would not be optimal for really big datasets, as the CSV format has a limit of rows in which can be opened at once, so if the number of rows exceed this value it may cause some delays in the processing of the model. For future versions of the package an option to just store internally all the values will have to be implemented to circumvent this issue. In the end the CSV files that will be created are soil parameters, precipitation, base evapotranspiration, minimum temperature and maximum temperature.

The last function, and the main one, is called "Spatial_AQC ()", its aims to read all the CSV files which were created from the spatial input data in the last function, run the AquaCrop model calculation, with the AquaCrop plugin, gather all the created outputs for each of the different pixels of the analyzed area and compile then in different CSV tables and raster files. Some of the outputs that the model can give are crop yield, evapotranspiration, runoff, drainage, biomass, irrigation needed and others. There are as well two different types of outputs that the model can provide, the seasonal ones that consider a value for the whole length of the simulation and daily values.

The way in which AquaCrop plugin runs the model calculation is that it reads all the information that are on the specific text files for the different parameters, the path for the files is set in the project file, and with that information it can create the seasonal and daily output file for that specific set of input parameters. The way in which SpatialAquaCrop approaches this is that it considers each of these runs as one of the pixels present in the raster, and it calculates everything necessary for that pixel and saves the output in a vector. Utilizing a for loop, this calculation is done for each of the different pixels of the raster and all their output data is saved into different vectors and in the end all those vectors are transformed back into the same raster format of the input data.

The seasonal outputs and daily outputs that are currently set in the final script are focused on water management/transportation and some crop related outputs. There are other outputs in which AquaCrop plugin can output, in which in the final version of the package, in which will be submitted to R to be implemented to its CRAM, will have the other outputs added as well. Besides the outputs in which the model can give, one last function was added to the last script, which is to calculate the green water footprint for the simulation, this was added due to the importance of this concept for different types of research that focus on the relationship between crop and water (Hoekstra et al., 2011).

The project for building this package started a few years ago and since then the AquaCrop plugin had an update which changed how some of the text files are set and their formatting. Due to this change, a small restructuring of the package is required, which will be done in the future for other planned research and papers and for the final submission of the package for the R CRAM. The scripts which were used in this thesis are currently available at github (SpatialAquaCrop, 2022) and when necessary, they will be update until everything will be contained in a package format and an overall overview of the package can be seen in figure 10. One important point to take note is that throughout this thesis SpatialAquaCrop will be mentioned as a package even though it has not been officially accepted as a package yet, that will be done for facilitating how it will be reference in the next chapters of this thesis.

Table 1. Input and output of major R functions within the SpatialAquaCrop package

FUNCTION	INPUT	OUTPUT
Initial_AQC	If the model will run utilizing :Field management, Groundwater table or Irrigation; If pre-determined crop files will be used or if they will be manually filled	Different .csv files depending on what the model will use to run and a data_fill.csv which has to be filled.
Control_AQC	The filed Data_fill.csv file; Soil texture; saturated hydraulic conductivity; field capacity; wilting point; soil water content at saturation; precipitation; maximum temperature; minimum temperature; reference evapotranspiration	Different .csv files containing all the soil and climate data; General Input text file that is AquaCrop plug-in uses to run the model;
Spatial_AQC	The climate and soil .csv files;	A .tif map of the seasonal and daily outpts;csv files of the selected daily outputs

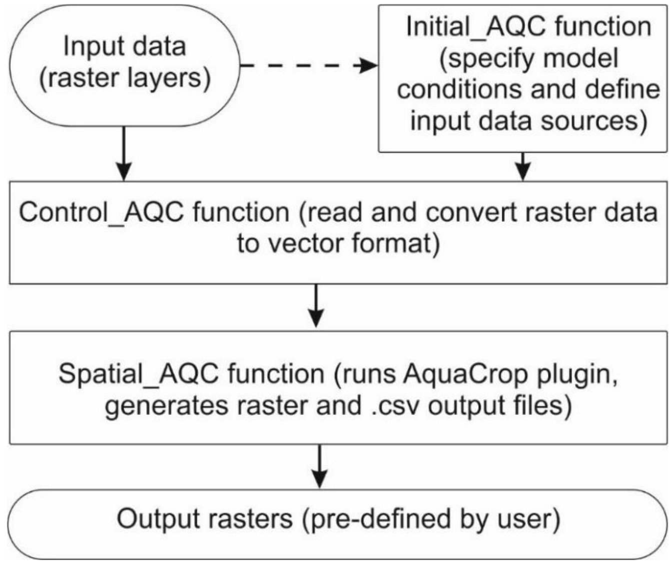


Fig 10 - Basic overview of the SpatialAquaCrop simulation

4.2. First case study

During the length of this PhD research different approaches with different aims were done while utilizing AquaCrop model and more specific the SpaticalAquaCrop as a methodology for simulating different crops in different scenarios (with a focus on water management, more specifically soil moisture). Some of these study cases ended up being presented in a scientific journal (Barros et al., 2022) and others in different scientific conferences, some of the study cases were not published but they are still relevant for the overall research progress of this PhD research progressed. This thesis will be divided into five different study cases, with explaining their objectives and methodology first, with later their results and discussing those results afterwards. The methodology applied for each study case has a striking similarity to one another, which is to use the SpatialAquaCrop package as its main tool for simulation and analysis.

The first case study aim was to verify how well the SpatialAquaCrop package performed while analyzing the output for two different crops, maize and sunflower, in a small catchment area in Hungary. There was no focus on what was analyzed for this simulation, but still some important results were seen in this study case, which helped to cement the analyses and study cases that came after this one.

For this case study the study area was the Rákos stream watershed, in Pest County, Hungary. Rákos stream is the main river in this study area, it mainly passes through agricultural areas and some urbanized areas as it flows in the direction of the Danube. The stream itself is 44 km long, with 187 km^2 catchment area, flowing from the Gödöllő Hills southward (Figure 11) that turns west to flow into the Danube River.

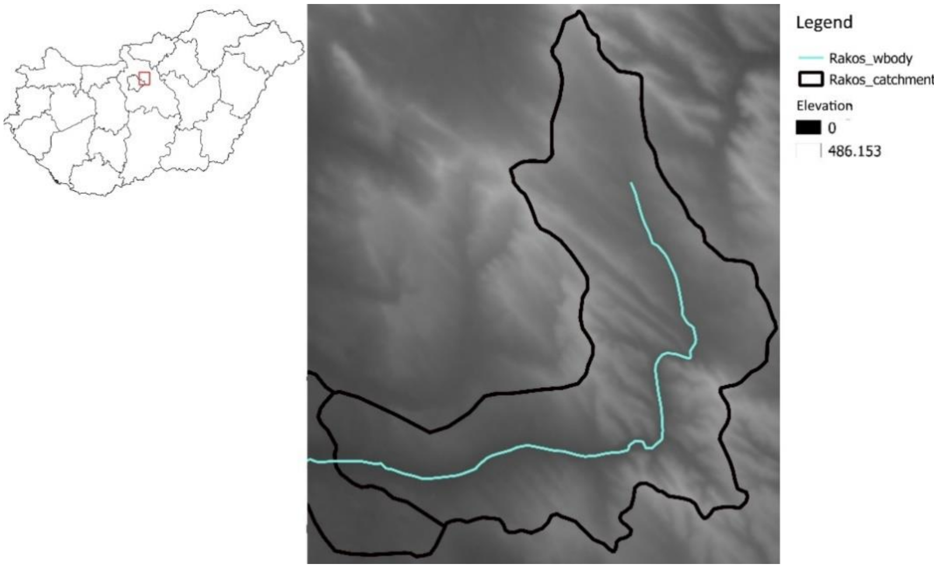


Figure 11 - Elevation map of the study area (EU-DEM)

Half of the stream's length (22 km long) flows through the capital city (Budapest) changing some of its characteristics as it passes through urbanized areas (Wahyuningsih et al., 2020). Throughout its history many changes were made to the stream and its surroundings, one of those major changes was that in the XVIII century the riverbed was controlled to avoid flood damage (Wahyuningsih et al., 2020). This helped to isolate the ecology of the river from the wider environment around it (IRN,2005; Saedi et al., 2020).

As mentioned before this study focused on running the SpatialAquaCrop plugin for two different crops for the whole of the study area, these two crops were maize and sunflower as they are crops which are commonly used in the region. For the input parameters that were chosen, the soil parameters were obtained from the CORINE dataset (Corine ,2023) with 6 data for 6 different depths of soil (0, 5,10, 15, 30 and 60 cm depth). The crop parameters were taken from the database that the AquaCrop software provides; for this analysis the climate data used was considered from just a particular point, the climate station at the research field at MATE university in Godollo (Barros et al., 2022), this way the variation in the results will mainly come from the soil parameters; no irrigation was considered, so the simulation ran only considering rainfall, no specific groundwater input was used so in this case the simulation considers that there is no shallow groundwater present in the system; no initial conditions were set; no field management practice was set and the simulation ran for the entirety of the 2020 year. These settings are the most basic in which SpatialAquaCrop can run its simulation, emphasizing again that the goal for this case study is to be just a demonstration of the capabilities of the SpatialAquaCrop package.

4.3. Second case study

For the second case study, the same area of the Rakos catchment was selected for the study, but for this one both soil and climate parameters had a spatial variation. The main goal of this study was to access first how the AquaCrop model can perform if not considering that the simulation area is a crop field but a grassland and second to access the soil moisture dynamics in this grassland scenario and then compare the results with point-based data that was gotten from the climate station at the research field for the MATE university on Godollo.

The first main point of discussion for this study case is the change of a crop field, in which the AquaCrop model was initially built for, for a grassland field. For this a change in the type of crop and its parameters are needed, for that some research was done and it was found that there are some studies that have already accomplished this type of "crop" In AquaCrop (Holzworth et al., 2015; Snow et al., 2014]) but mainly the study done by Kim and Kalurachchi (Kim and Kaluarachchi, 2015) in which he utilized alfalfa as a crop for a grassland simulation.

As discussed before, the parameters that are set in the crop file, which the AquaCrop plugin utilizes, dictate what are the crop characteristics and how it will be affected by the climate and soil parameters, so a custom crop file must be created and for that the studies of Allen (Allen et al., 1998) were followed, and a custom alfalfa crop was created. To simulate a grassland alfalfa was selected and its parameters were changed so that it could resemble the best to a grass in a grassland, for example the canopy cover growth of the crop was changed to resemble the closest to one of grass. A set growing cycle of 275 days (starting in in March) was set as well.

Talking a bit more of the study area, even though it is almost the same as the previous case study, the area has different types of land cover, which can be seen in figure 12 which was based in the 2018 CORINE (Corine ,2023) land cover dataset (Corine ,2023). In 2018, about 32% of the area was covered by artificial surfaces (such as urban or industrial areas), 35% by agricultural land (including pastures), 31% by forests and semi-natural habitats (including natural grasslands) and 1% was covered by wetlands (Saeidi et al., 2019).

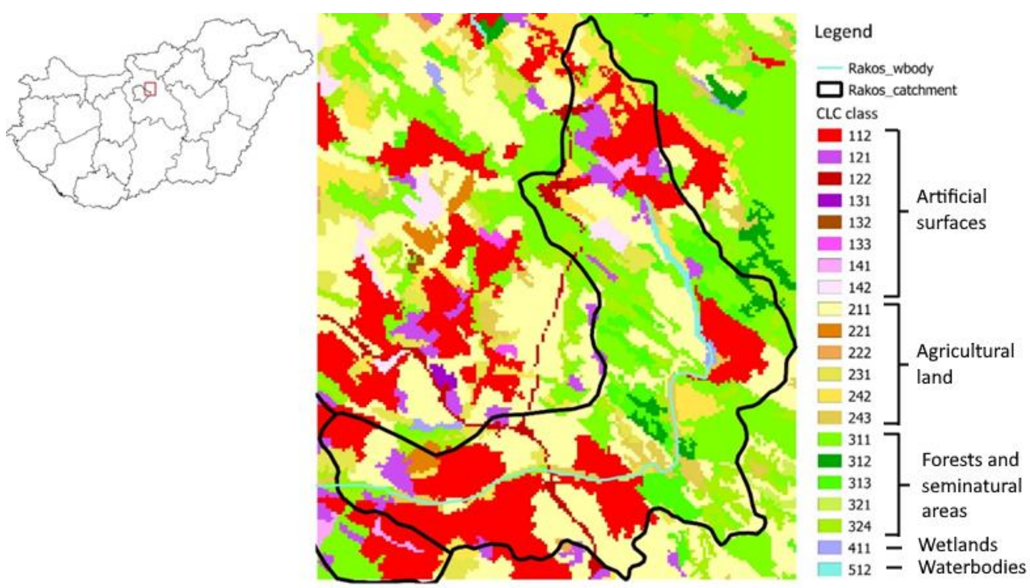


Figure 12 - Land cover of the area based on the 2018 CORINE Land Cover dataset (Corine ,2023)

The input data for this simulation was obtained from different sources. Soil data was accessed from two sources, field capacity (FC), saturation (SAT) and permanent wilting point (PWP) data were downloaded from EU-SoilHydroGrids ver1.0 (with 250 x 250 m spatial resolution), while soil texture data was derived from the DO-SoReMI.hu initiative (Pásztor et al., 2015) (with 100 x 100 m spatial resolution). Even though these two sources have different resolutions, the one with 250 x 250 m resolution was resampled to match the 100 x 100 m spatial resolution. Different depths were considered as well, for this study the different soil depths that were taken in consideration for the simulation were: 0, 5, 15, 30 and 60 cm. Figure 13 presents the spatial variability of soil texture of the top 30 cm layer within the study area.

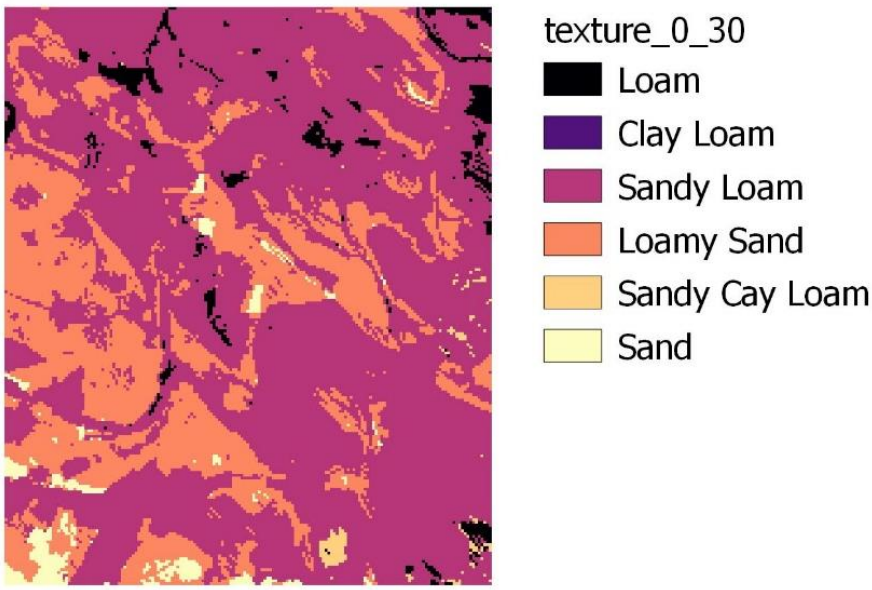


Figure 13 - Texture map up to 30 cm soil depth.

The climate data (daily precipitation, maximum and minimum temperature) used in the simulation was accessed from the Meteorological Data Repository of the Hungarian Meteorological Service (OMSZ). Daily potential evapotranspiration has been calculated using the Pennman-Monteith equation (Allen et al., 1998). One software which facilitates the calculation of potential evapotranspiration is the ETO Calculator (Allen et al., 2001), which is available to be downloaded at the FAO website. One advantage of utilizing this software is that the end results already output the result in the proper text file format which is used by the AquaCrop Plugin and the SpatialAquaCrop package. Climatic data was available at a 0.1˚ x 0.1˚ spatial resolution and was interpolated and resampled to the target 100 x 100 m grid.

For the other parameters necessary for the simulation the standard values, which are provided by FAO, and come in example files with the AquaCrop software have been considered. The simulation ran from 1st of March of 2020 to the 30th of November and no initial conditions or field management was considered in the run.

For the final comparison of the simulated results with field based meteorological data, a limited time series from the meteorological station situated at the experimental field of MATE University in Gödöllő, Hungary has been utilized. The parameters that were taken from it were precipitation and soil moisture content.

4.4. Third study case

After analyzing the results for the second case study it was seen that the soil moisture results for AquaCrop seemed to have a higher variation than what was expected, even though it is know that results from simulated models suffer from a higher variation when compared to field data (Huang et al., 2022). There are different options in which could be chosen to approach this issue, for this small study case a comparasion between the results of soil moisture for Aqucrop and Hydrus model has been done and for the final study case the quality of the input parameters was chosen as a focus to try to improve the quality of the soil moisture results.

For this small study the main objective was to compare the soil moisture values obtained from the AquaCrop and Hydrus model and analyze how they behave in comparison to each other. Both simulations ran for the year of 2020 and 2021 and the selected location for the analysis was the meteorological station at MATE university in Godollo. This simulation was done while taking in consideration the same input data for both models, soil parameters were based on the 2018 CORINE (Corine, 2023) land cover dataset and the climate parameters were taken from different sources for each of the years, for 2020 it was from OMS (OMS, 2023) and for 2021 from the data captured by the meteorological station located at the research field. The crop chosen was wheat, as it is a common crop grown in the region. The simulation ran for the entirety of both years.

4.5. Fourth study case

Further down on the research timeline for this PhD thesis, while having a better understanding of the AquaCrop model and reformulated the SpatialAquaCrop package into what would be the final stable version that would be used in this PhD research a new study case was proposed to keep analysing how well results from AquaCrop model can be used in different scenarios and keep presenting the efficacy of the ability of SpatialAquaCrop to process spatial datasets.

As one of the main goals of this thesis is to show the application of AquaCrop model in a raster format applied within the R environment (SpatialAquaCrop package), for this study case first a point-based validation was carried out for soil moisture for a maize field in Martonvasar, Hungary, for 2020. It was possible to gain information on the performance of the model under initial settings having no site-specific parametrization, as the area in Martonvasar can be considered a data scarce area. Besides this validation a comparison between modelled biomass and green canopy crop cover against NDVI was done for winter wheat at an experimental site in Gödöllő for the year of 2020 and 2021, this comparison was done for the growth period until around its senescence. As field scale yield information is considered to be sensitive data it is difficult to obtain from farmers, hence NDVI was used as a proxy for biomass in the validation years. Following the validation efforts the developed

SpatialAquaCrop package (Fay et al., 2023) was used to simulate wheat growth for the year of 2020 and 2021 in the Rákos watershed region for the comparison with NDVI.

Point-based evaluation of the AquaCrop model was carried out in two different sites, on a maize field in Martonvásár for surface soil moisture, and in the experimental field in Gödöllő (which is located inside the Rákos stream catchment) an NDVI comparison between modeled biomass and green canopy crop cover (CC) for winter wheat was done. Specific soil, climate and crop data were taken in consideration for each of the sites for a better parametrization of the model.

For biomass and CC comparison, soil parameters locally analyzed and meteorological data from the local meteorological station (situated at the experimental field for the MATE university, Gödöllő, Hungary) has been utilized (precipitation, temperature) and from that reference evapotranspiration was derived utilizing the Pennman-Monteith equation (Allen et all., 1998).

Crop parameters for winter wheat and maize (for the Martonvásár site) were mostly kept the same as the standard ones provided in the AquaCrop software (for the modeling), just the length of the days between sowing to emergence, maximum rooting depth, senescence, flowering and maturity have been changed, in accordance to Szász (Szasz, 1988) and winter wheat at the site (Gödöllő) was sown on 1st of December and harvested on 23rd of July .

First NDVI index was calculated utilizing equation 6.

$$\boldsymbol{NDVI} = \frac{\boldsymbol{NIR - RED}}{\boldsymbol{NIR + RED}} \tag{9}$$

For this comparison Sentinel 2 images were used to calculate NDVI, in specific band 8 for NIR (near infrared) and band 4 for RED (red).

After NDVI, biomass and CC results were calculated, they were plotted against one another to check for correlation, for that coefficient of determination (R^2) and correlation coefficient were calculated. Statistical significance for the correlation coefficient was checked afterwards as well with the Shapiro-Welch t-test. This comparison was not made for the whole length of the simulation (sowing until harvesting), just until the crop’s senescence, which for winter wheat in Hungary is around the beginning of June. This length was chosen because chlorophyl concentration diminishes during senescence (Hörtensteiner, 2006), lowering the NDVI value while biomass and CC still have a growing trend.

As for the validation at the Martonvasar site, the necessary soil and meteorological data for running the AquaCrop model has been provided by the work of Sándor (Sándor et al., 2020). The maize field trial was established at Martonvásár, under ploughing and minimal tillage managements in 2020 aiming at the effect of cover crops sawn for the winter period. The plot size is 35 m x 17.5 m for each treatment. The treatments are set up in two replicates. The used maize (Zea mais L.) on the field of the trial was sowed under conventional ploughing without cover crop (i.e. the control treatment of the trial) as it represents the most typical management in the region. The chernozem soil of the experiment is non acidic loam with deep A horizon with 1.96-2.26 m% humus content. Maize was sown on 16th of April and harvested in 21st of October. Soil parameters for the modeling were obtained using field data on soil physical properties and water retention.

Even though these validations and analysis were done in a point-based approach, SpatialAquaCrop package was still used for it, as at this point with the addition of the possibility of extracting daily outputs from any dates and as well extracting the whole timeseries results for selected parameters, the package presents as a good alternative for the AquaCrop software for simulating point based data, while not having the proper visual features that the AquaCrop software has, as it fully built in an R environment, it can be quite beneficial for the researcher utilizing this package, as it can expedite the process of analysing the different outputs that the model creates.

4.5. Fifth study case

After the different study cases it was possible to prove the efficacy of the SpatialAquaCrop package and how well it can handle spatial (raster in .TIF format) and point based data. Still one issue that was present in the different prior results is that the soil moisture results that were obtained with the AquaCrop model simulation had most of the time higher values than the ones checked in the field, and the intensity in how the daily variation of soil moisture behaved was more intense as well when compared to the results in the field, this intensity is expected as simulated data tend to vary more when compared to data collected in the field (Huang et al., 2022). It is known that AquaCrop model has been validated in many different studies (Huai et al., 2019, Barros et al., 2022, Rakotoarivony et al., 2020), so in this case it is not the model that is decreasing the accuracy of the results but rather what is thought is that the quality of the input data may be interfering with how accurate the results are. This point will be taken in consideration when analysing and coming up with the last study case.

For the last study case of this PhD, different points in the South part of Hungary were chosen (29 different meteorological stations in the middle of agricultural fields) in a point-based approach to compare the surface soil moisture near different meteorological stations with the soil moisture results while utilizing the AquaCrop model and the SpatialAquaCrop package to process the points. The meteorological stations are located in different agricultural fields, but the stations themselves are usually separated from the crops and most of the time surrounded by grass. The image bellow show where the stations are located in Hungary (Figure 14). OVF provided data for several meteorological stations throughout all of Hungary, but for focused research a cluster station at the south of Hungary were chosen for this study.

The stations for this case study are mainly located in the Bács-Kiskun County and the Danube-Tisza Interfleuve, which is one of the most drought-prone regions in Hungary (Meyer et al., 2017). Some characteristics main characteristics of the Danube-Tisza Interfleuve is that there has been a decrease in the groundwater level for the past years, due to different effects such as change in climate patterns (droughts) and channelization of rivers (Molnar et al., 2018), and a change and degradation of the natural vegetation in the area (Biró et al., 2008).

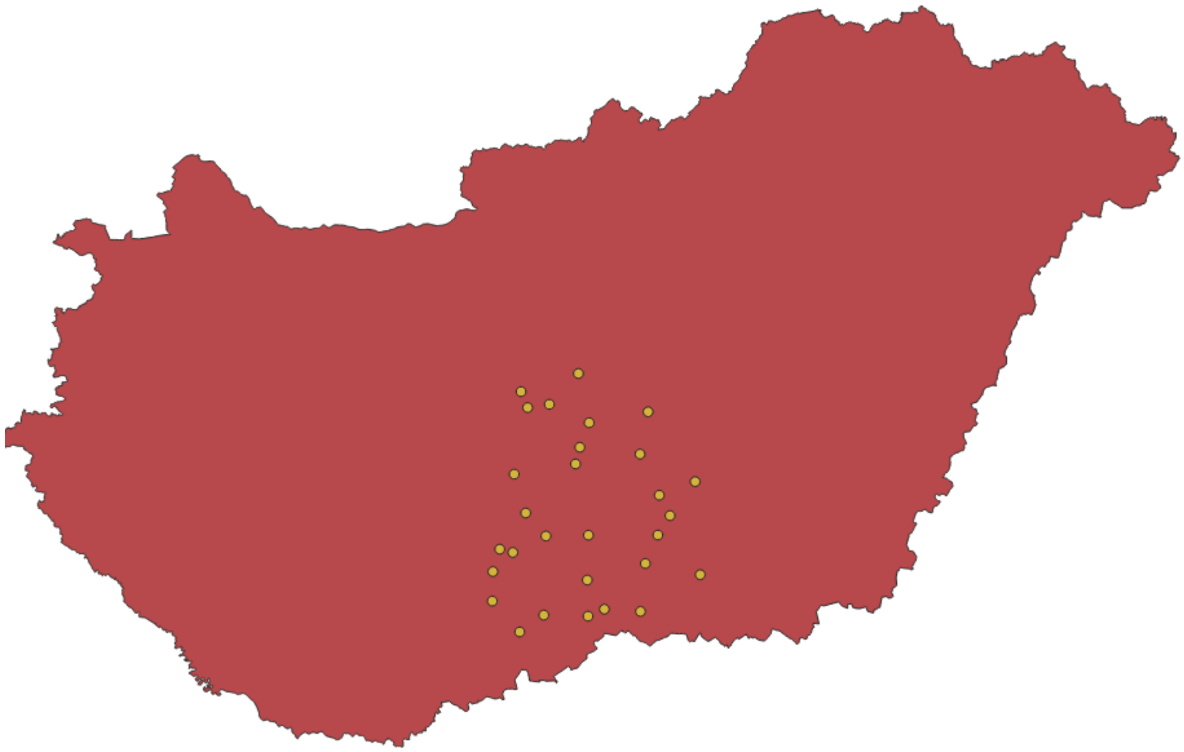


Figure 14 - Location of the meteorological stations within Hungary

The input data for the simulation run were obtained from different sources, the meteorological data was obtained from the different meteorological stations provided by OVF, this data included daily precipitation, maximum and minimum temperature from 2020 to 2022. Evapotranspiration was later calculated utilizing the ETo calculator (Allen et al., 2011), which can be downloaded from the FAO website and as prior mentioned the result from the software is already in the format in which both AquaCrop software and SpatialAquaCrop package can utilize.

Soil parameters were taken from different raster sources, there were three sets of crop parameters that were used in this study case. The first set of parameters (Field capacity, permanent wilting point and soil saturation) were taken from EU-SoilHydroGrids ver1.0 (with 250 x 250 m spatial resolution) and the texture was derived from Corine dataset (Corine, 2023) and this texture was compared to the standard Ksat values that AquaCrop provides (figure 42) and the Ksat values taken from it. The other set of values were obtained from (HUN-REN, 2024) which provided all soil parameters needed for the simulation. The third set of parameters is a mix from the Ksat from AquaCrop and other soil parameters from HUN-REN, as HUN-REN dataset does have a different texture classification, following USDA texture reference (USDA, 2024), so this texture was as well compared to the standard Ksat values from Aquarop (figure 42) and the related values were used for each of the analyzed points. For the initial runs 100% penetrability and 0% of gravel was considered (the same way for the prior simulations for the other study cases). The exact soil parameters for each of the stations were not available at the time of the study and processing of the data, as it was mentioned prior as the different soil data grid sets were generated with mathematical models, but at the moment OVF has released at https://vizhiany.vizugy.hu/ a new dataset with a in-depth soil description of the different areas where the station are located, providing a different, and in theory, a more accurate dataset that could be used in future researches.

As the meteorological stations are located in closed areas with a high possibility of grass covering the soil, it was chosen again to run the simulation while utilizing a crop file that tries to simulate grass. The base values for the simulation were taken from the work of Terán-Chaves for Ryegrass and of Raes and Kim for alfalfa, taking in consideration these works (Kim and Kaluarachchi, 2015; Allan et al., 1998; Terán-Chaves et al., 2022) a new set of parameters was created for this study case. Even though the crop parameters which have been utilized in these studies can simulate the growth of two different types of grass quite well, for this study some further modifications were needed for the crop parameters in the crop file, so that the main goal of comparing the soil moisture in the soil close to the meteorological stations with the simulated on in AquaCrop could be achieved.

As AquaCrop utilizes a base evapotranspiration for its calculations, which is the evapotranspiration from a grassy field, this way it can be assumed that the soil moisture that has been obtained from a grassy field can be considered as base soil moisture for the region, or in other words a soil moisture values that has not been influenced by the different crops or vegetation in the region. Being able to simulate such value is quite beneficial as it can help to understand better the water movement in the region and help with flood prevention (Terán-Chaves et al., 2022).

Knowing that and utilizing the crop parameters from the two mentioned papers as a base (Kim and Kaluarachchi, 2015; Allan et al., 1998; Terán-Chaves et al., 2022) this new crop was "created", in which it will be referred as "New Crop" from now on. This new crop was designed in a way in which senescence would take almost all its length to start and maximum rooting depth would be achieved in a few days, this way forcing the model to consider that the crop is present and fully grown throughout most of the year length in which the simulation happened. These parameters for the calendar days of the new crop can be seen bellow on table 2.

Table 2 – Calendar days setup for the "New Crop"

0	Calendar Days: from sowing to emergence
4	Calendar Days: from sowing to maximum rooting depth
214	Calendar Days: from sowing to start senescence
285	Calendar Days: from sowing to maturity (length of crop cycle)

.

No optional parameters were chosen at first for the simulation, but after the first results were checked, some of these parameters were added to try to achieve the best simulation results.

The first goal for this analysis was to compare how well AquaCrop would model surface soil moisture in these specific points, while validating the model results with surface soil moisture results that were surveyed in these points, while utilizing raster based data as an input. The simulation ran from 2020 to 2022 and considered that the "New crop" started its growth cycle in March of 2020.

5. RESULTS AND DISCUSSION

5.1. Study cases results

5.1.1. First study case results

As mentioned before, only the soil input parameters were considered as a raster for this simulation, due to this the variability of the different outputs in which the model can create are highly dependent on these parameters. The results in raster format that were obtained in this simulation were: drainage, runoff, evapotranspiration, infiltration, crop yield and green water footprint. Bellow it is possible to see different maps, figure 15 to figure 20, in which R could create utilizing the raster output (.tif format) that was produced by the package, meaning that these results could be read by any GIS software.

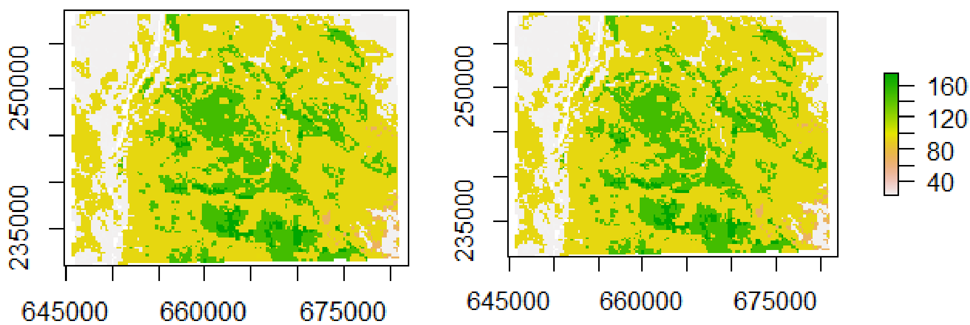


Figure 15 - Drainage (mm) map for maize (left) and sunflower (right)

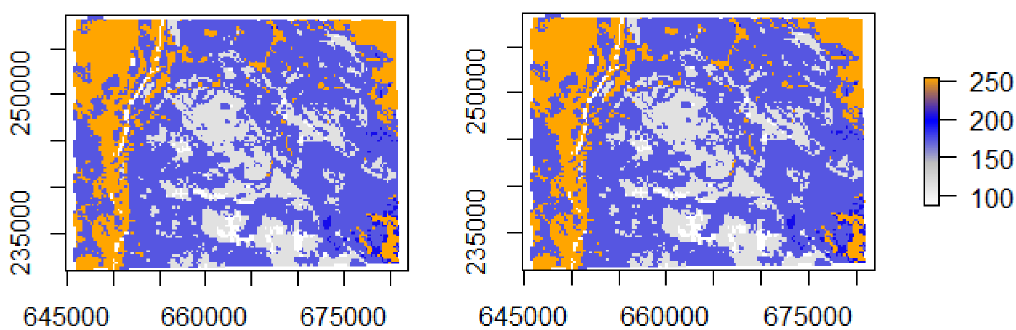


Figure 16 - Runoff (mm) map of maize (left) and sunflower (right)

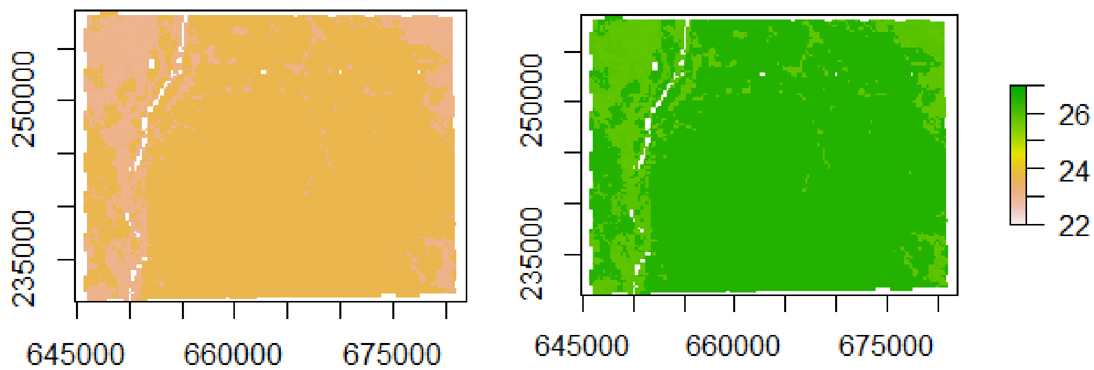


Figure 17 - Evapotranspiration (mm) map of maize (left) and sunflower (right)

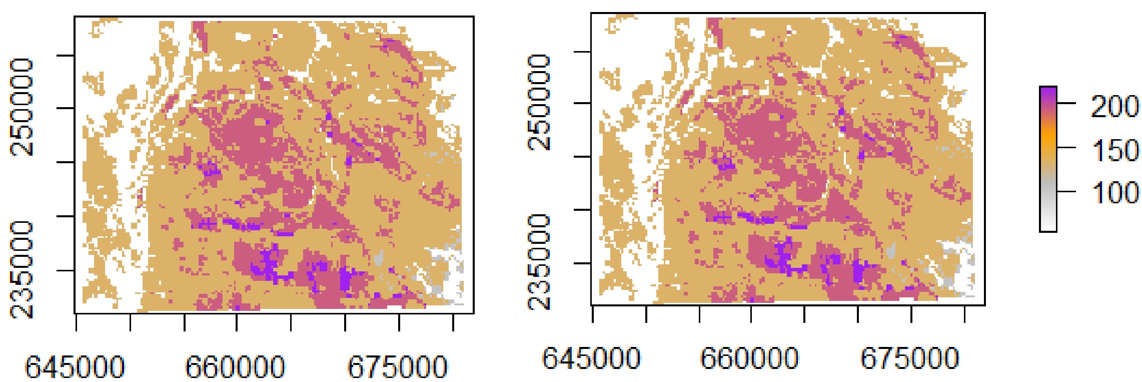


Figure 18 - Infiltration (mm) map of maize (left) and sunflower (right)

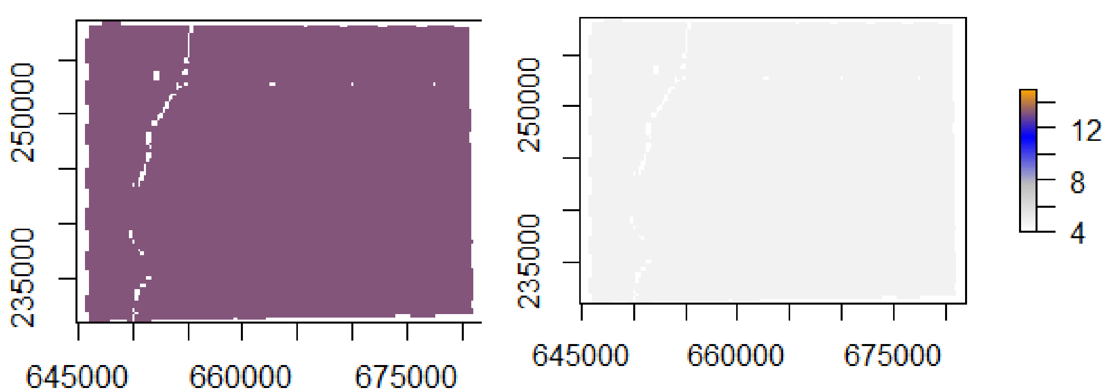


Figure 19 - Crop Yield (ton/ha) map of maize (left) and sunflower (right)

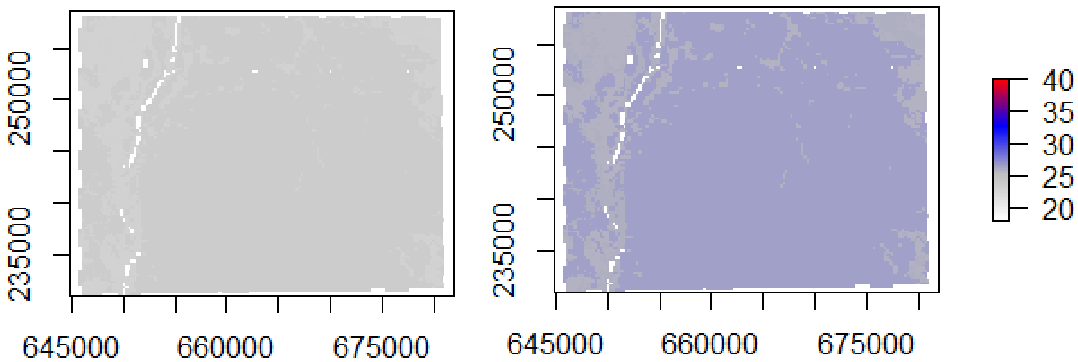


Figure 20 - Green water footprint (m^3/ton) map of maize (left) and sunflower (right)

Even though the only spatial results that were used in the simulation were the soil parameters, the first results that were obtained in this simulation are pertinent. First it is clear that all the functions in the package worked as the simulation could run without any issue from the beginning to the end and produce the different outputs that it was set to produce. As a note, at this point of the package development only the seasonal outputs were set as a produced result, but in versions created afterwards of this study case daily outputs are present. As soil is the only spatial variable it is possible to see how differently it affects the output parameters showing the strength in how these results correlate to the change of soil parameters.

Analyzing figure 15 and 16, drainage and runoff it is possible to see that they are inversely correlated, so in the area where drainage is at the highest runoff is at the lowest, which makes sense as where it was more difficult for the available water to infiltrate, it would be lost as runoff. Figure 17 shows the different in evapotranspiration for each of the crops, there is a small different in it because of the soil spatial variation but the main difference is because of the two different types of crops, with sunflower having the higher one compared to maize, which this can be seen in some studies that compared both crops (He et al., 2024). Figure 20, for green water footprint, shows a small spatial variance as well and the bigger one is with the different of crops, having sunflower have a higher value for green water footprint, around 25 m^3/ton, than maize, around 23 m^3/ton, this reflects well with data seen at the water footprint network (Water footprint network, 2023). Another main difference between the crops is their yield (figure 19), maize shows a higher yield, around 12 ton/ha, and sunflower around 6 ton/ha.

5.1.2 Results second case

The first results to check are the results from the seasonal outputs in which AquaCrop Plugin generated and SpatialAquaCrop transformed into raster format files. These seasonal files take in consideration the whole simulation period and not the result of only one day. Figure 21 shows the seasonal results for infiltration, runoff, evapotranspiration and biomass for the area.

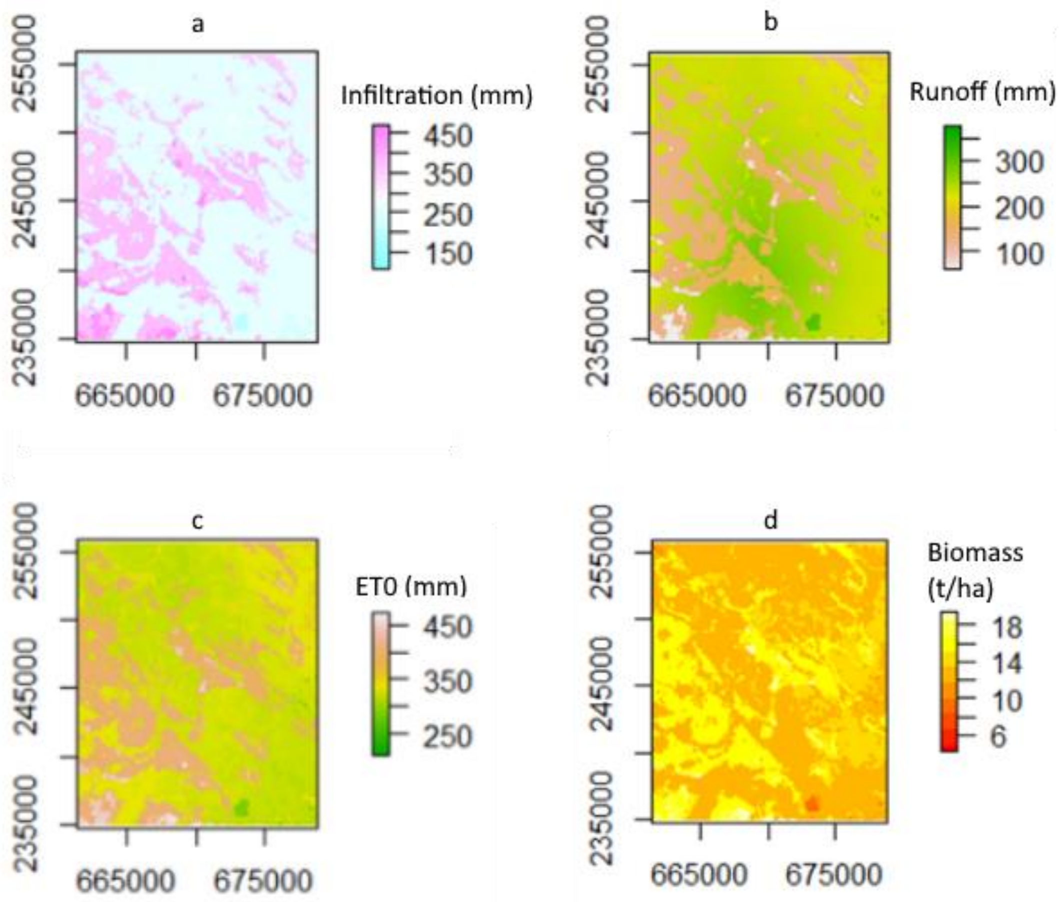


Figure 21 - Spatial variation maps of seasonal Infiltration (4.a.), Runoff (4.b.), Evapotranspiration (4.c.) and Biomass (4.d.).

Runoff and infiltration (Figure 21a and 21b) show some correlation between them, as it is to be expected as when more water able to infiltrate, less is available to be lost to runoff, so when infiltration values are low the runoff values in that region are higher, which that clearly shows that the soil spatial variability for the area was taken into consideration. This spatial variability clearly shows the spatial heterogeneity of the area. However, in this scenario (also limited by the applied model), the effects of topography and surface conditions (such as ruggedness) have not been considered for the infiltration and runoff values. But according to Vereecken et al. (Vereecken et al., 2016) this approach can have benefits, too, since the very detailed local parameters are usually not representative enough for the whole modeled environment.

Biomass results are as well relatable to infiltration, as in areas which infiltration is higher biomass values are higher as well. This is seen in the study of Meron et al. (Meron et al, 2007) as he draws a correlation between water infiltration and biomass density of plants. Another correlation that can be seen with biomass is the correlation between biomass and evapotranspiration, in which where the biomass value is high, a high result for evapotranspiration can be seen as well. This is shown at the study of Tolk and Howel (Tolk and Howell, 2009) in which this correlation is presented as well.

As mentioned before there was one new feature that was introduced in the version of the SpatialAquaCrop package which was used for this study case. From this version forward it is possible to save the values of the daily output results of the several parameters in which the AquaCrop plugin output. For this study case two different parameters were chosen to be shown, daily water content for the rooting zone (at 60 cm) and percentage of relative evapotranspiration. One particular day of the simulation was chosen at random (10th of September) for presenting these daily outputs, which the spatial variation of these parameters can be see in figure 22 for the specified date.

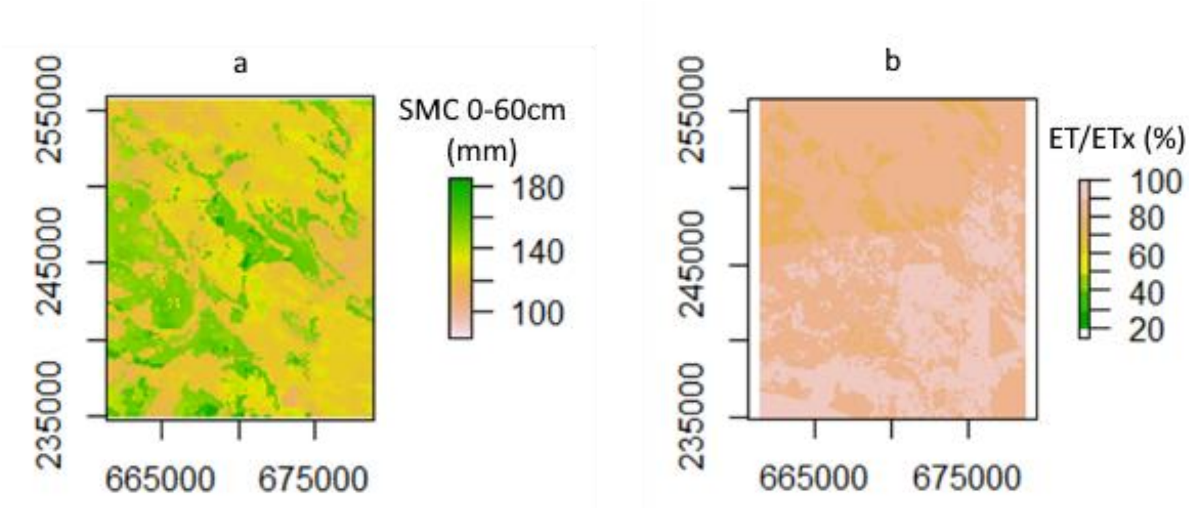


Figure 22 - Spatial variation maps of daily water content for the rooting zone (5.a.) and percentage of relative evapotranspiration (5.b.) for the 10th of September 2020

The ability to output daily results in a spatial format greatly enhances the capability of the SpatialAquaCrop package, resulting in a great addition to the package. Due to this it is possible to analyse the results of the simulation as a time series, which was done for this study case. One of the goals of this study case was to compare simulated soil moisture from the AquaCrop model with field soil moisture values, in a way to validate the results obtained with the simulation.

For analyzing soil moisture for the region, a comparison with some of the model inputs and outputs was done with daily data from the monitoring station that belongs to the MATE university in the city of Gödöllő, Hungary, checking see how well the simulated data relates to field data from a monitoring station. This issue has been also investigated by Hungarian researchers, like Kozma et al. (Kozma et al., 2019), Móricz et al. (Móricz et al., 2012).

Figure 23 presents an overview of the time series of daily data for that specific point (or the related 100 by 100 m grid cell) for soil moisture content, canopy cover, mean temperature and precipitation. The results show that the generated outputs (soil moisture and canopy cover) are clearly dependent on the input data (temperature and precipitation), as expected from the AquaCrop model. Soil moisture is inversely related to the canopy cover for most of the simulation time that changes around the middle of august, where there is a big precipitation event which leads to a "saturation" of the soil for the rest of the simulated period. As the average temperature decreases, the canopy cover decreases as well, showing that the simulated grassland cover decreases due to the lower temperatures.

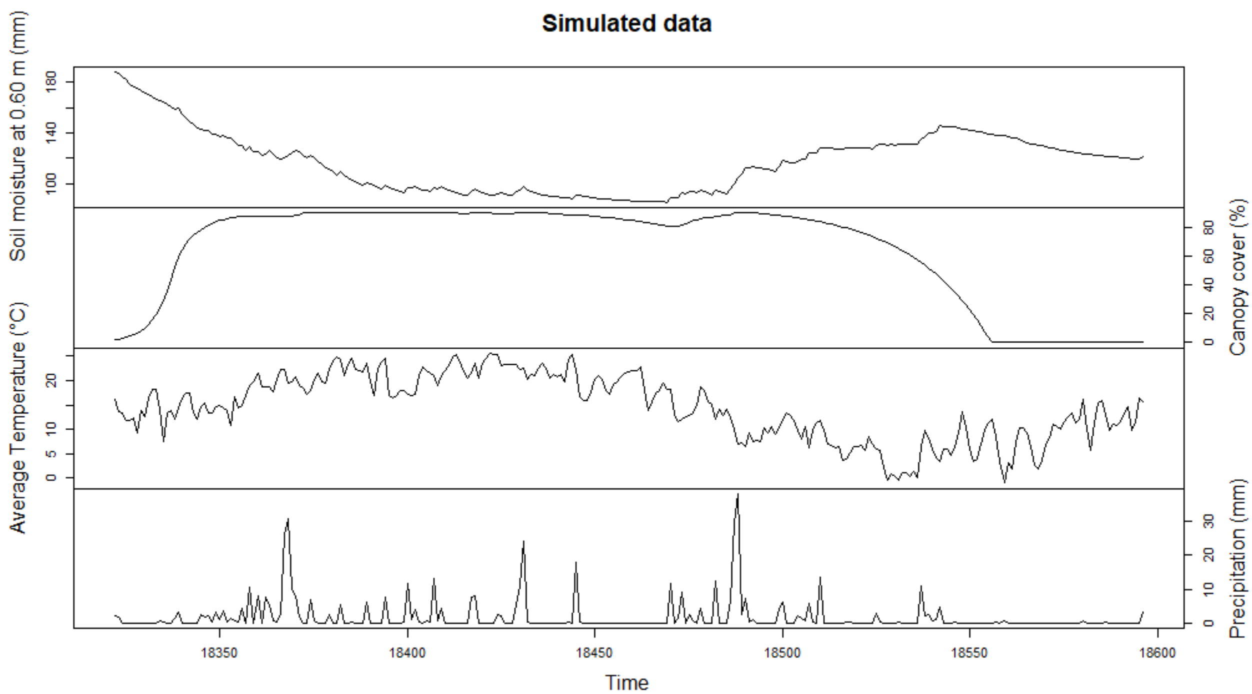


Figure 23 - Comparisons of different outputs from the AquaCrop model

One point that had to be taken into consideration when making this comparison is that the meteorological station which has been used for this study had been just established at the time of this study case and because of that data was only available from the end of July 2020, so just a portion of the timeseries could be used for the comparison.

Figure 24 presents the comparison of precipitation input data (based on an interpolated country level dataset) with the rain gauge data collected at the meteorological station, presenting a clear alignment of precipitation events, with a significant correlation value of 0.86, meaning that the precipitation data used in the simulation was on par with the precipitation data gathered at the meteorological station.

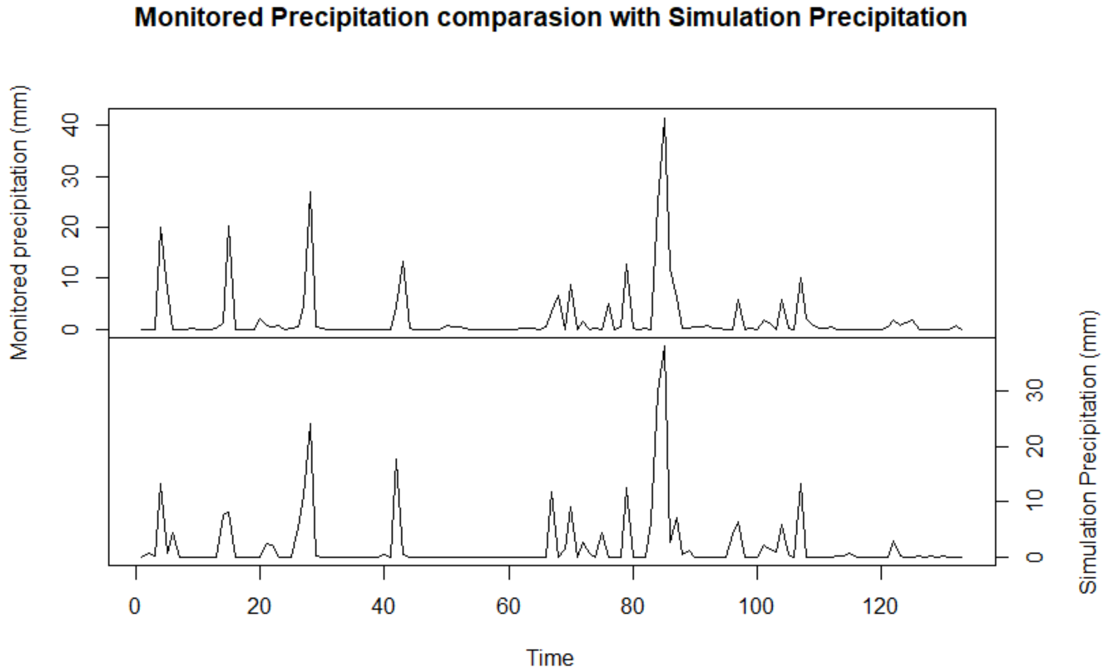


Figure 24 - Comparison of the simulated precipitation data with the field monitored ones

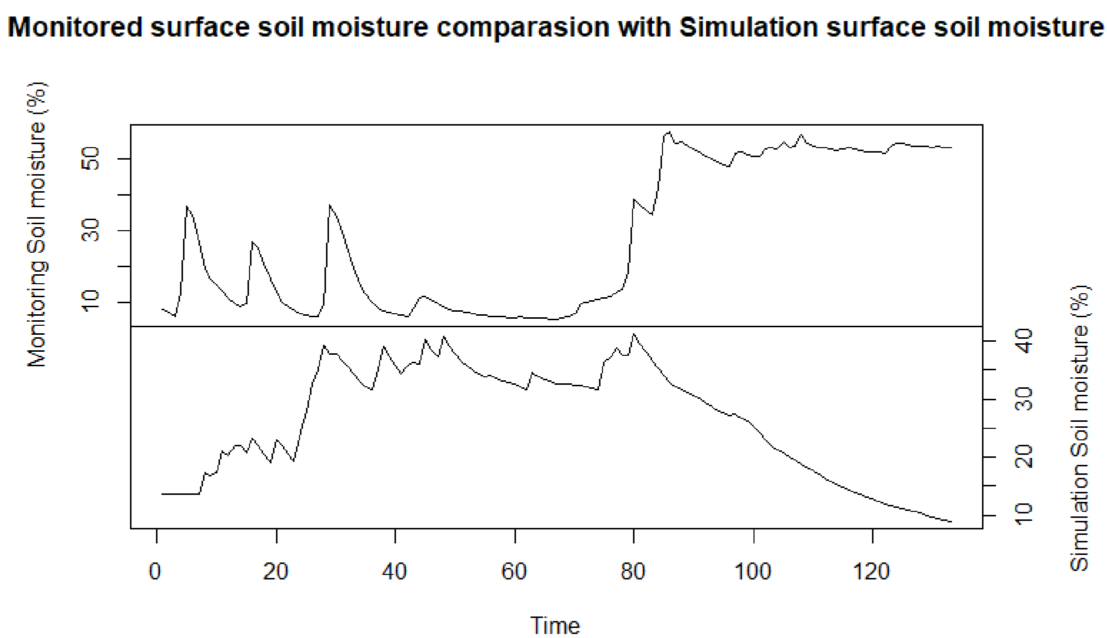


Figure 25 - Comparison of the simulated soil moisture content (surface layer) data with the field monitored ones

Comparison of soil moisture content (Figure 25) however does present a clear difference between the monitored and modeled soil moisture content values, especially from the middle of October when the soil moisture on the field stays at a constantly high value while the simulated value drops until being close to 0. It is important to point out that the simulated data shows a lower variance than the field values. This will be seen in another study case as well, but the reason of this different and how to improve it will be addressed at that point.

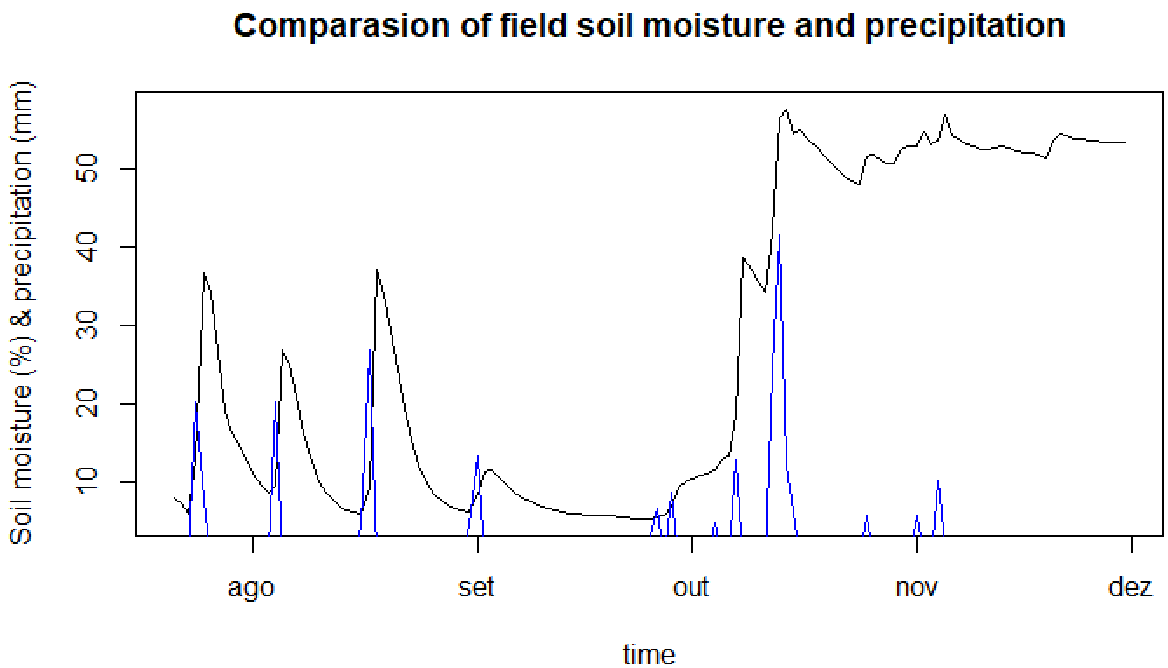


Figure 27 - Field (measured) soil moisture content for the surface layer (black) and precipitation (blue)

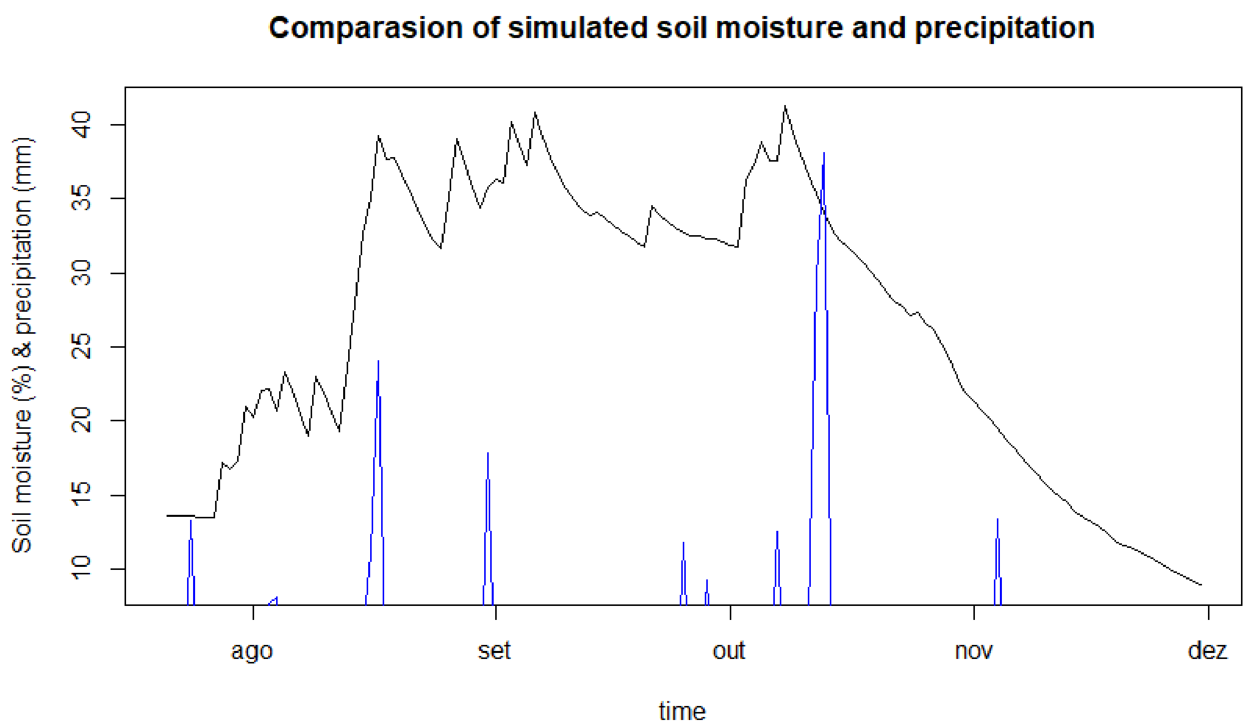


Figure 28 - Simulated soil moisture content for the surface layer (black) and precipitation (blue)

Figures 27 and 28 present a comparison of precipitation data and topsoil soil moisture content for measured and simulated data respectively. The rise in measured soil moisture for the middle of October (Figure 28) happens at the same time as a big precipitation event occurs and after that the soil stays in a "saturated" state until the end of the time series. Before October both Figure 27 and 28 soil moisture peaks follow the precipitation peaks as well, but Figure 27 shows an overall lower variance, which could mean that other inputs (such as soil parameters) are making this difference between the two graphs occur, since precipitation is practically similar between them. This soil parameters assumption will be checked more in depth in the final study case of this thesis (as mentioned in prior paragraphs) and it will be seen that changing these soil parameters will make the simulated results fit better with the ones present in field.

5.1.3 Results third case

For 2020 (Figure 29) both AquaCrop and the Hydrus modeled results react in a similar way to the precipitation intensity, having similar patterns throughout the year. Both have similar values in the middle of the year and when crop growth is happening. In the beginning and end both of their values have a considerable change in intensity, but still reacting with the same pattern.

Figure 30 shows the modelled soil moisture with Hydrus and the soil moisture results obtained at the research field on site. It is possible to see that the results do not match, just having a bit of the same reactions for the precipitation. AquaCrop wasn't considered in this comparison, as the results that were gotten from it were not satisfactory. It was found afterwards that some climate parameters given by the meteorological station had some issues in their readings, which caused some unintended variation on months with lower temperatures (winter and part of autumn).

An overall result that can be seen for the two years is that the results in AquaCrop have in general higher values as results when comparing to Hydrus, and the results in AquaCrop have a higher response to climate variations, especially regarding precipitation. That may be caused by how the AquaCrop model utilizes the soil parameters in its mathematical equations for the simulation (Raes et al, 2018).

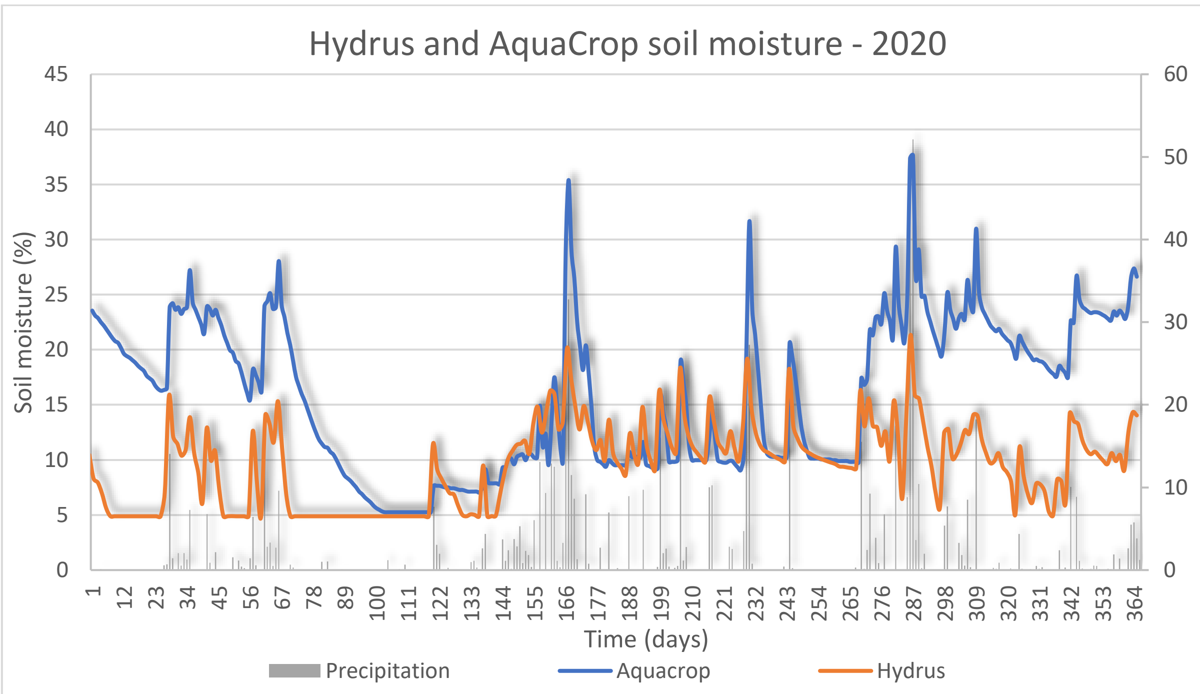


Figure 29 - Hydrus and AquaCrop Soil moisture - 2020

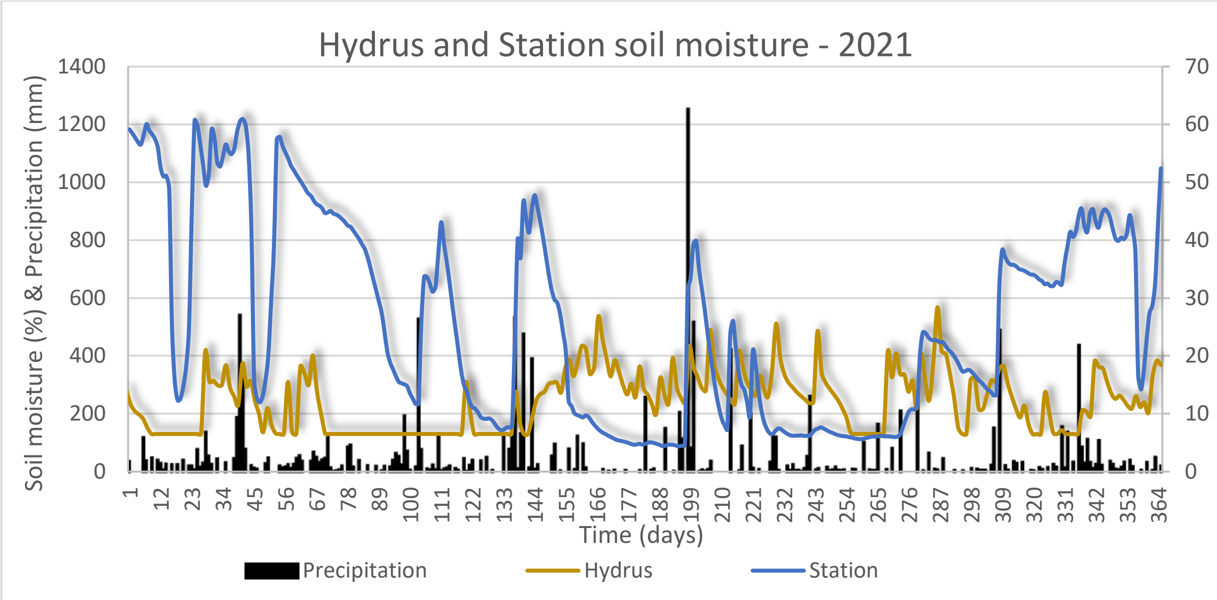


Figure 30 - Hydrus and Research station Soil moisture – 2021

5.1.4 Results fourth case

First it was evaluated how the NDVI index relates to modeled biomass and green canopy crop cover (CC) and if there is a correlation between them. This was done for winter wheat for the years of 2020 and 2021 at the experimental site in Gödöllő.

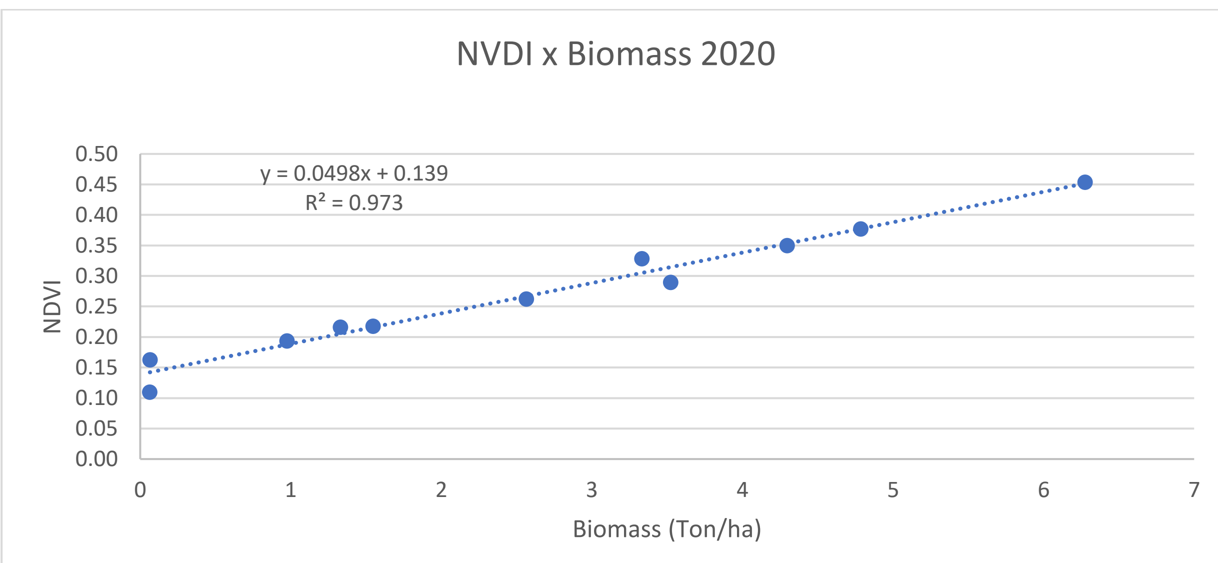
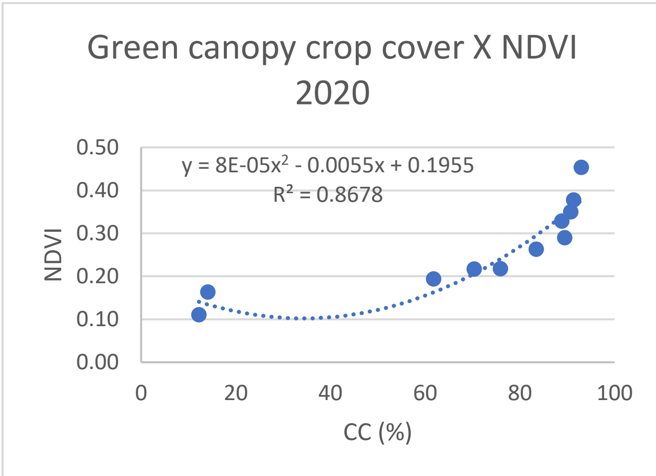


Figure 31 - Comparison between NDVI index and modeled biomass for winter wheat in 2020



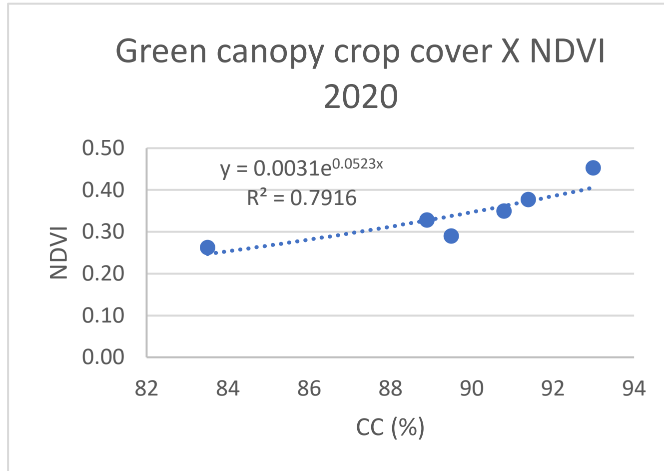


Figure 32 - Comparison between NDVI index and modeled green canopy crop cover for winter wheat in 2020 while: (32.a.) Considering the whole time series; (32.b.) Considering just when green canopy crop cover is above 80%.

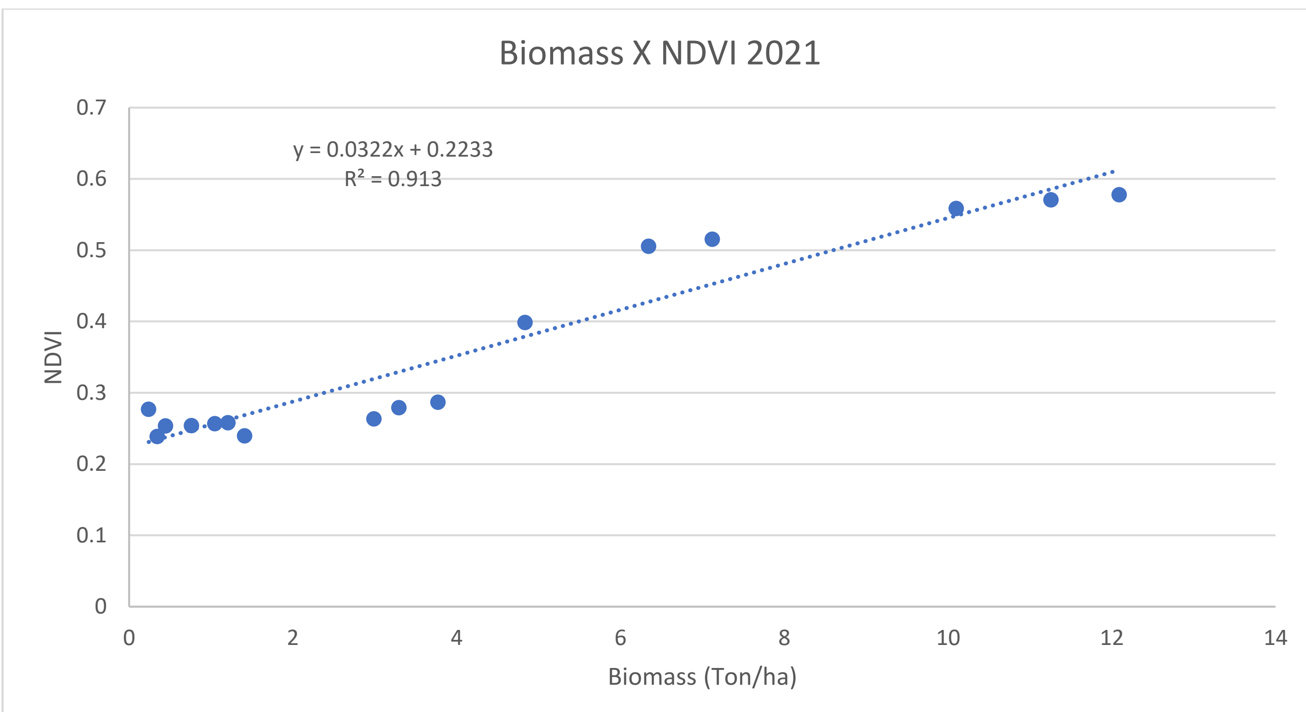


Figure 33 - Comparison between NDVI index and modeled biomass for winter wheat in 2021

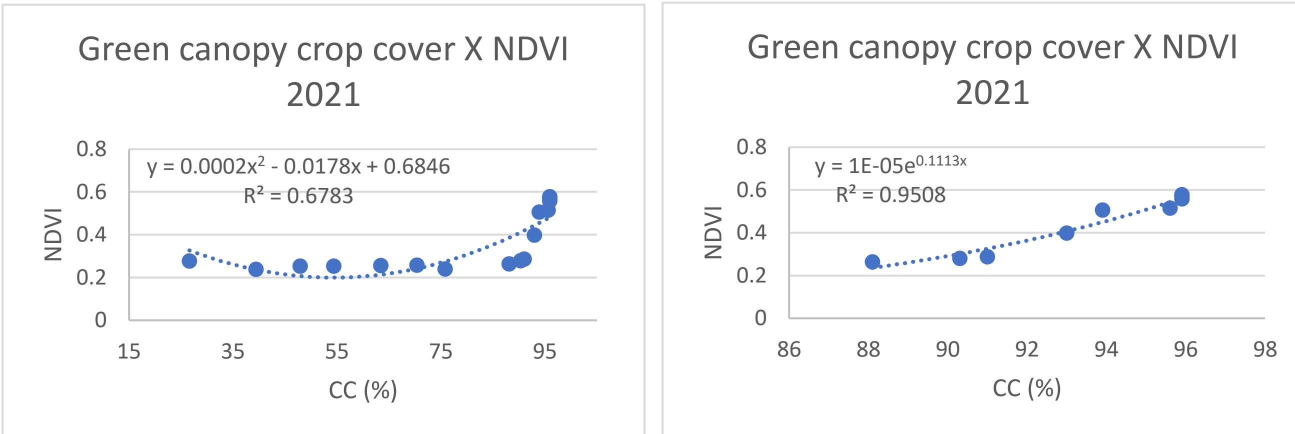


Figure 34 - Comparison between NDVI index and modeled green canopy crop cover for winter wheat in 2021 while: (34.a.) Considering the whole time series; (34.b.) Considering just when green canopy crop cover is above 80%.

Figures: 31,32,33 and 34 show the different comparisons and the different years which were considered. One important difference from both years is that in 2021 there were more available dates to calculate NDVI due to weather conditions in the region. Because of that, in 2021 the comparison is done until the beginning of senescence and for 2020 the last suitable quality satellite data was available for the beginning of May. Szabó et al., 2024 have found that UAV-based NDVI values generally higher in irrigated areas than in non-irrigated ones.

In relation to biomass, both years show a visible correlation between both parameters and a good R^2 value for both (Figures 31 and 33). Besides that, the correlation coefficient was checked for both of them. For 2020 the correlation coefficient was 0.83 with a p value of 0.02, showing significance. As for 2021 the correlation coefficient was 0.95 with a p value of 0.001 showing significance.

For green canopy crop cover a linear regression model was first used, but its R^2 was not satisfactory, due to an, close to, exponential growth of CC (green canopy crop cover) after 80% cover. As a result, a polynomial regression was the one with the best fit, having a R^2 of 0.86 for 2020 (Figure 32) and 0.67 for 2021 (Figure 34). When just considering the points over 80% CC it was seen that the best regression model fit changed to an exponential one, with R^3 being 0.79 (Figure 32) and 0.92 (Figure 34) for 2020 and 2021 respectively.

As for the correlation coefficient for CC, the correlation coefficient for 2020 was 0.80 with a p value of $1.53E^{-5}$, showing significance, and for 2021 the correlation coefficient was 0.65 with a p value of $1.25E^{-9}$, showing significance as well.

Figure 35 shows the difference between the modeled soil moisture and the soil moisture that was measured at the field in Martonvásár.

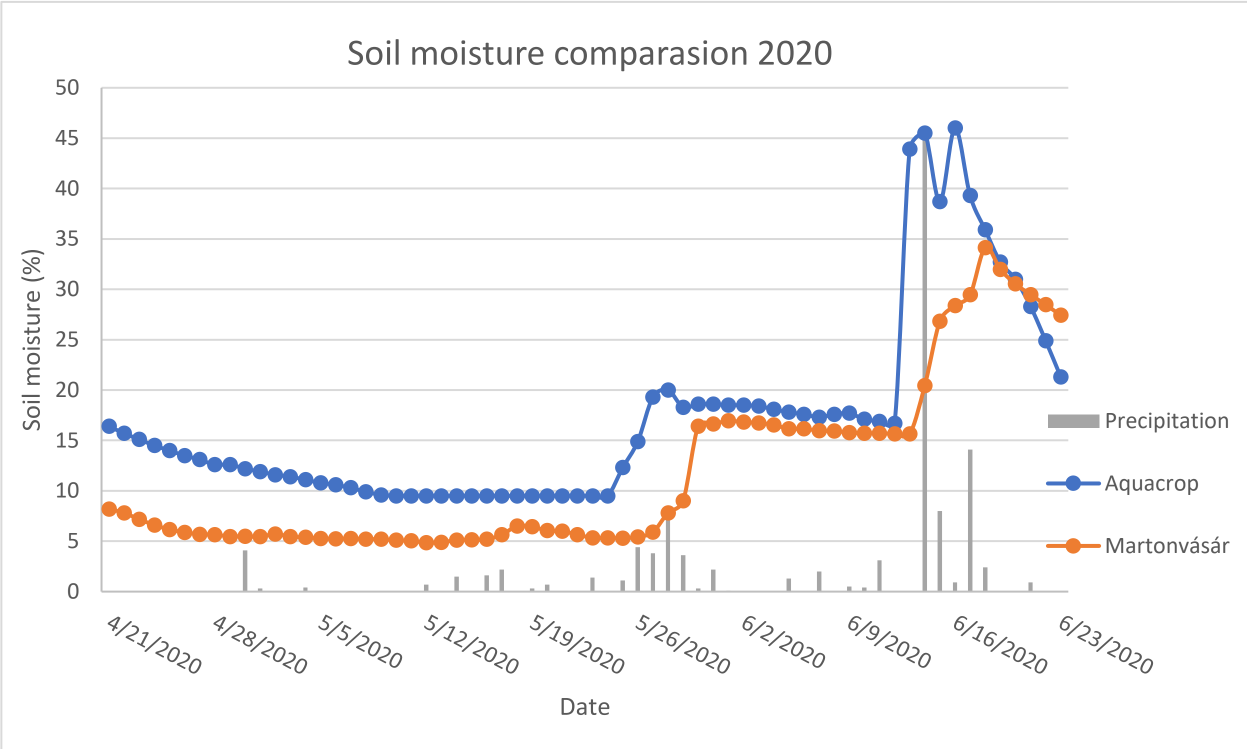


Figure 35 - Comparison between modeled soil moisture and measure soil moisture in Martonvásar for 2020.

Figure 35 presents the time series of modelled and measured soil moisture. The calculated correlation coefficient was 0.82. After that to check for statistical significance, we have applied the Shapiro-Welch t-test and its result was of a p value of 0.001, meaning that statistical significance exists. It is possible to see as well that after two “significant” precipitation events the values between the two timeseries start to change that the model error gets decreased, but this decrease doesn’t happen during the days which the precipitation events occurred, where the difference between them is the highest. There is a recurring detail in which happened for all of the soil moisture results that can be seen with AquaCrop in all the prior results of the study cases is that the soil moisture results react with a higher variance mostly due to precipitation values.

5.1.5 Results fifth case

When first analyzing the results for the different meteorological stations, it was possible to see that there was a big discrepancy in how soil moisture behaved for the different years. Another thing that was noticed was that there was quite a difference in the behaviour of soil moisture for the different analyzed points, with correlations between the modeled soil moisture and the surveyed one varying from values of 0.4 to 0.8. The results with low correlation values showed similar results to past study cases, in which the soil moisture had a higher daily variation and response to different precipitation events or sometimes opposite behaving from the surveyed soil moisture from the sites. Figures 36, 37, 38 and 39 show the different timeseries for different stations and different time frames.

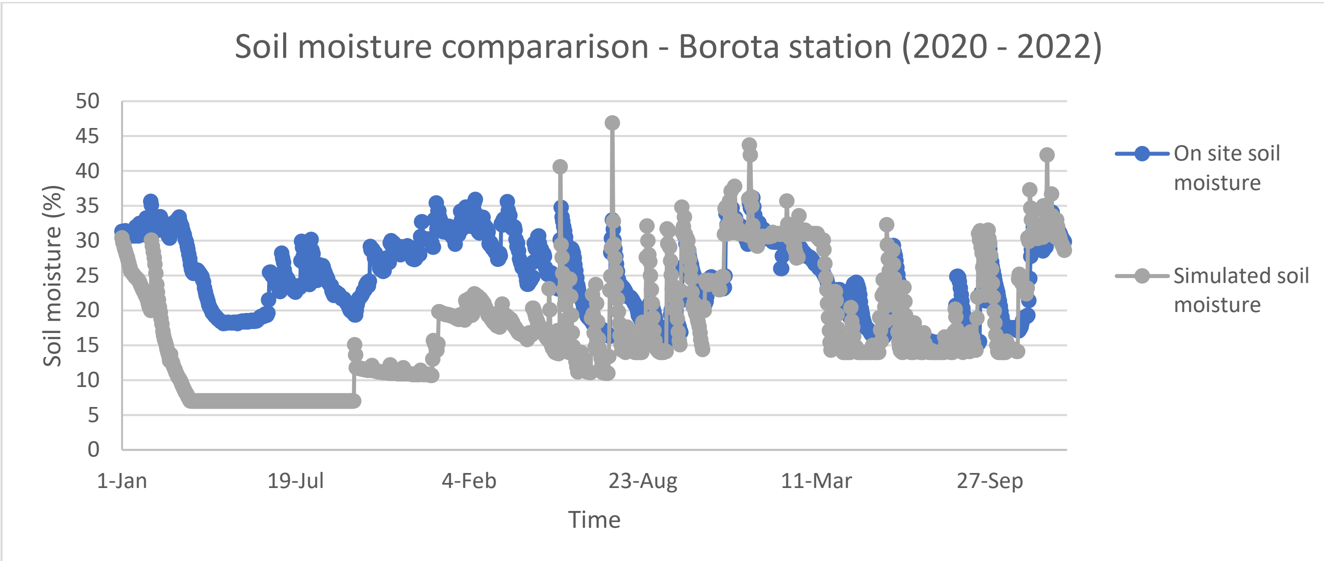


Figure 36 – Soil moisture comparison from 2020 to 2022 Borota

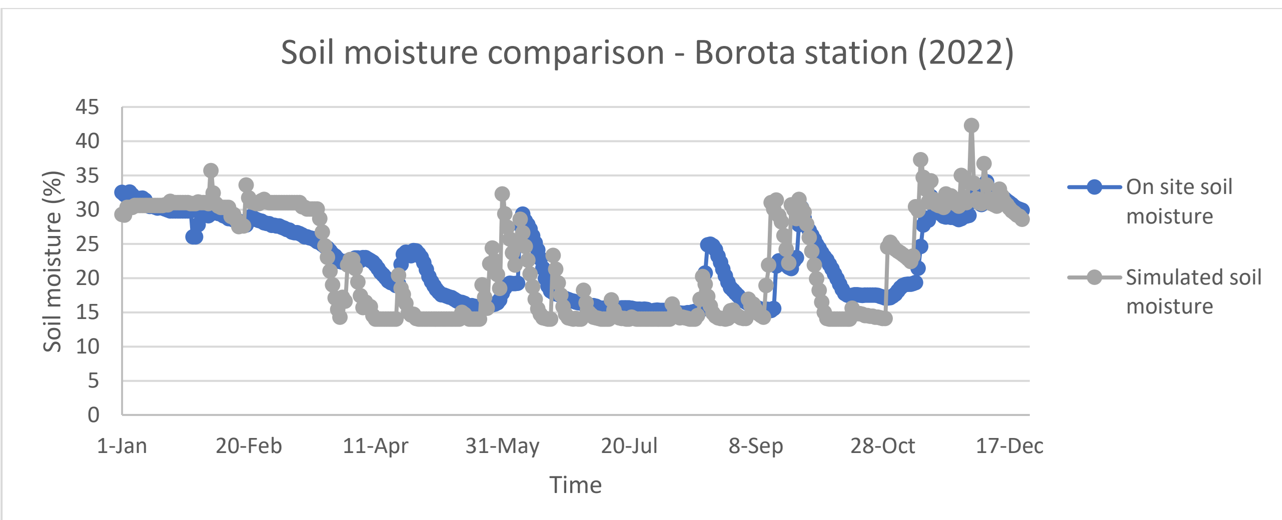


Figure 37 – Soil moisture comparison 2022 Borota

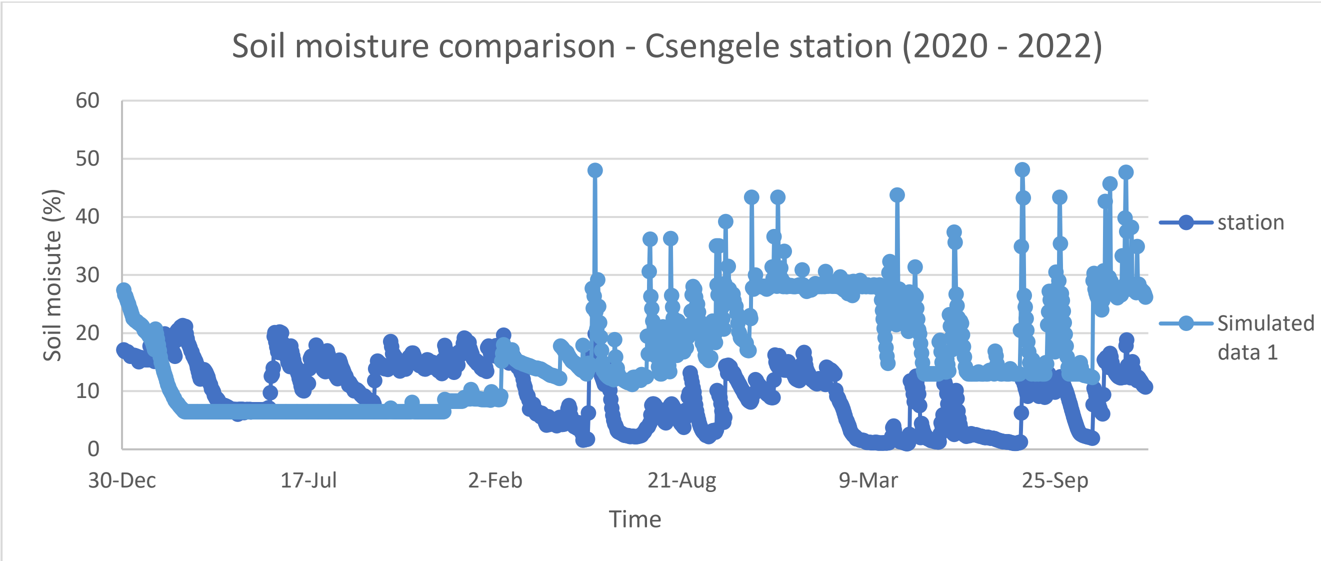


Figure 38 – Soil moisture comparison from 2020 to 2022 Csengele

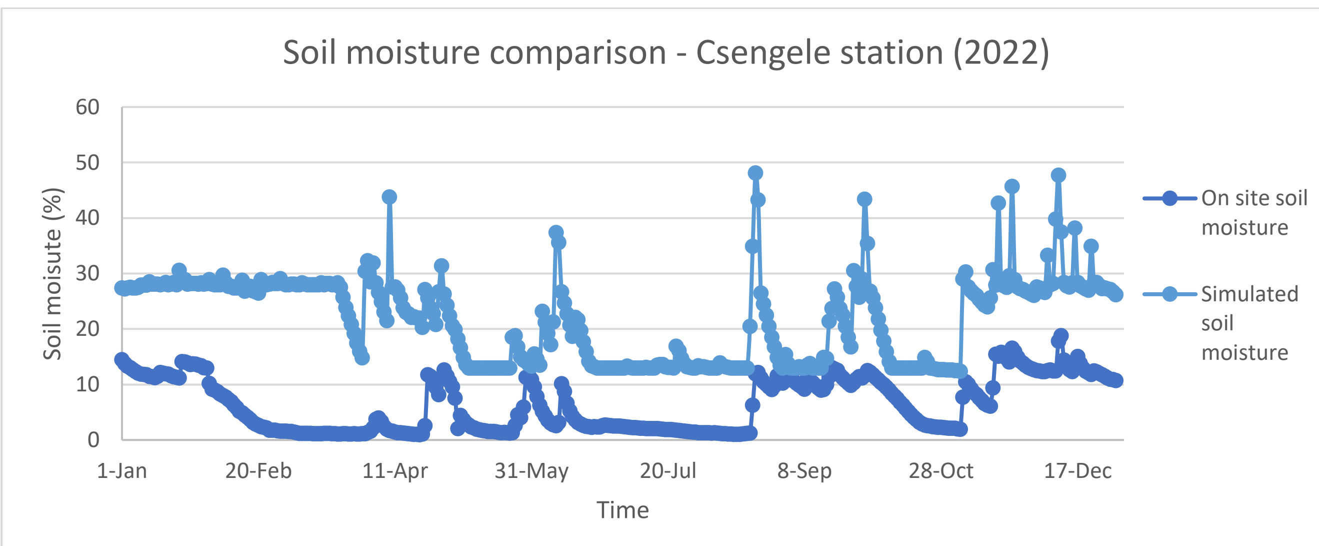


Figure 39 – Soil moisture comparison 2022 Csengele

As it can be seen in Figures 36, 37, 38 and 39 there is a difference from station to station, as the soil moisture parameters change from one to the other and how AquaCrop can simulate each point. Comparing the station in Borota and the station in Csengele results for the 3 years a big difference can be seen. For Borota de simulated soil moisture in the beginning has a lower value in the beginning and starting from the middle of the second year the values start to become closer to each other. The correlation value between the simulated and on site soil moisture for Borota is 0.40 when considering the whole timeseries (3 years) and 0.87 when considering just 2022. For Csengele the simulated soil moisture behaves a bit differently, being lower in the beginning of 2020 and then gradually having higher values than the on site soil moisture, having around 15% or higher difference between each other in soil moisture value. The correlation for this station was clearly lower, having values of -0.13 for 2020 to 2022 and 0.47 for 2022. This trend of having a better comparison between the two soil moisture for the year 2022 was seen for all the other simulated points as well.

Knowing that the best results could be seen for the year of 2022, the year was chosen to further continue this comparison study. Even though some of the station showed promising results with correlation values higher than 7.0, more than half of them showed correlation values lower than 7.0, not being satisfactory in theses cases. To improve the simulated soil moisture results, some changes in the soil parameters, and sometimes adding other effects such as mulching or the presence of groundwater in a specific depth, were made, so that the correlation between the modeled results and the onsite results would increase, having the the soil parameters being what mainly was affecting the difference in soil moisture results. These changes made the correlation between the two soil moistures for some of the points to improve up to around 0.15. Figures 40 and 41 shows the timeseries for the station in Csengele for 2022 after these changes were made.

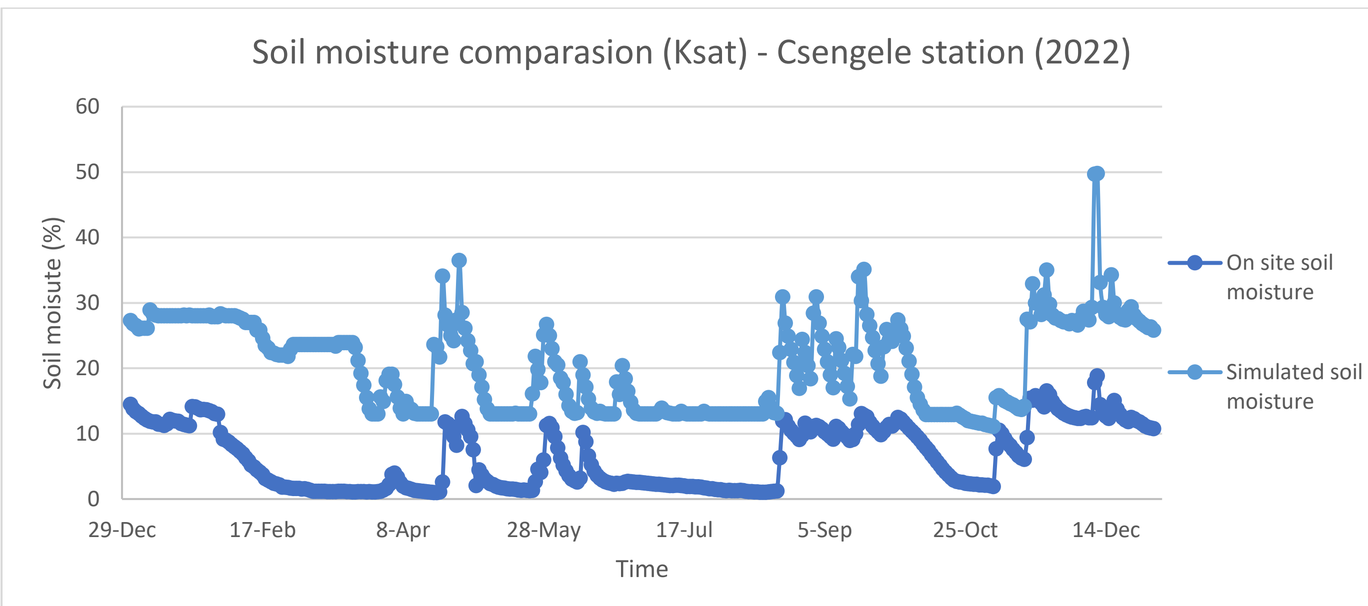


Figure 40 – 2nd Soil moisture comparison 2022 Csengele

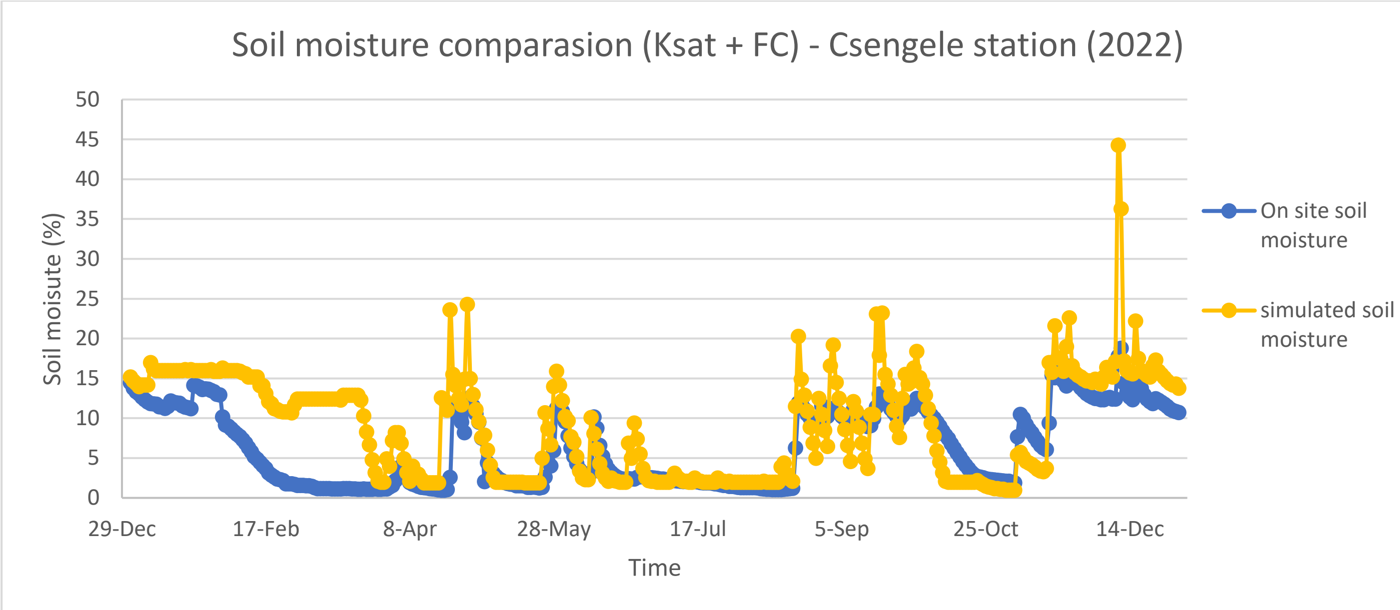


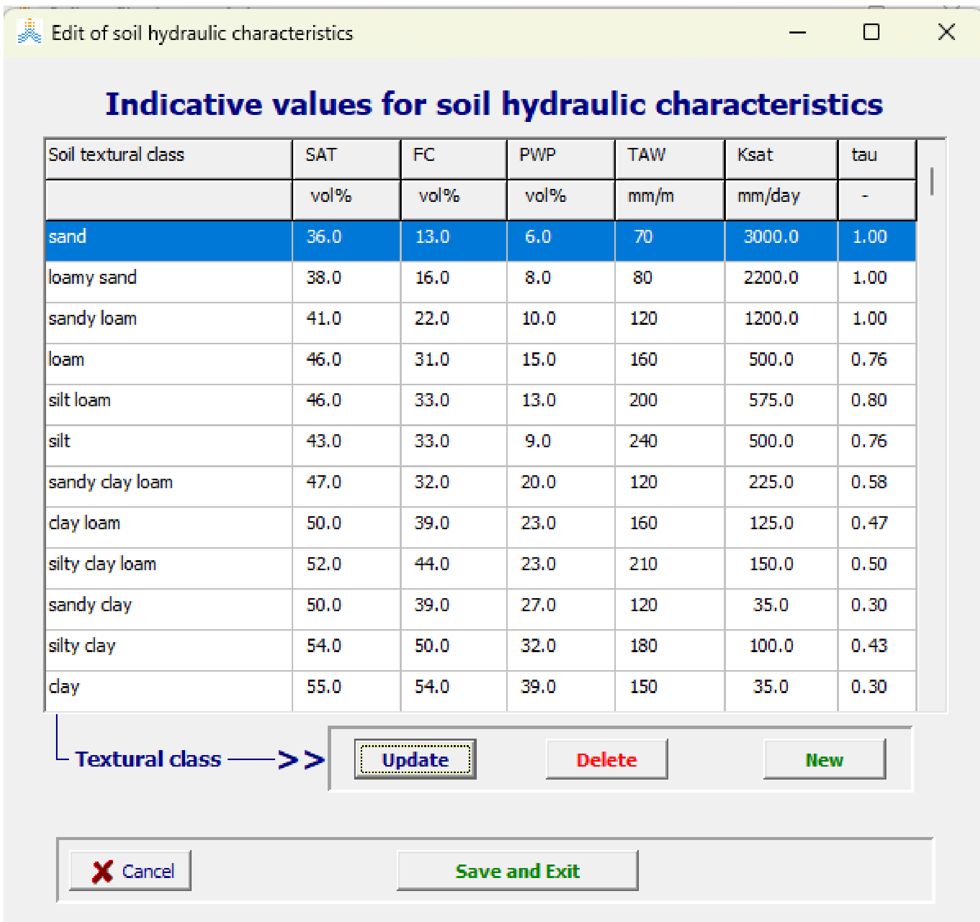
Figure 41 – 2nd Soil moisture comparison 2022 Csengele

First it was noticed that changing the Ksat would influence how the correlation between the two soil moistures would behave. In the case for Figures 40 and 41 for the station located in Csengele, the Ksat was changed from 3000 mm/day (value based on the texture raster, in this case sandy texture) to 500 mm/day (closer to a silt soil), because It can be seen in Fig 40 that the simulated soil moisture has a higher response for daily inputs (like precipitation) and changing the Ksat for a lower value made these daily variations closer to the one found on site (Fig 40). Similar changes for the Ksat were done for most of the stations that showed a correlation lower than 7.0 and in general showed improved results.

Changing the Ksat value made the daily variation from the simulated soil moisture be closer to the one found on site (Fig 40), but still there was a big different in between their values. For that difference to be lower a change in the Field Capacity (FC), generally close to halving the FC value, and considering the Wilting Point as the lowest value for soil moisture that can be seen on site. These changes can be seen in Fig 41 for the station in Csengeled and it can be visually seen that the difference in value between the simulated results and on site results are quite lower for most of the year, presenting only a bigger difference for colder periods. Mulching and a set depth for groundwater were checked as well in a way to improve the correlation results for this analysis, but even though changing/considering some of them for some stations would improve their correlation value, this was not true for all the stations, so it was chosen to leave them out of the changes for a preferred change that could be used for all station and would have a similar effect to them (soil parameters).

As mentioned, not every change in the Ksat would improve the correlation between the two soil moistures for the station, but it has been seen that changing soil parameters led to a better response when comparing both soil moistures. Because of that one important point that was checked was the table of indicative values for soil hydraulic characteristics (Figure 42). So when the Ksat was changed, for example from 3000 mm/day to 500 mm/day, if the standard values for the soil parameters (mainly

FC, SAT and PWP) that were obtained in the raster input files matched the table provided by AquaCrop, there would be a considerable improvement in correlation between the two soil moistures for the station, and if the soil parameters obtained from the raster input file had a bigger difference when comparing to the ones present in the table, the improvement in the correlation was not great or sometimes there was no improvement at all. Because of this, two questions were raised. The first is that if changing Ksat would actually provide an improvement for the results in some points and the second question is if the input raster that was used for texture/soil parameters actually had some discrepancies from the real parameters obtained at the different station locations.



Soil textural class	SAT	FC	PWP	TAW	Ksat	tau
	vol%	vol%	vol%	mm/m	mm/day	-
sand	36.0	13.0	6.0	70	3000.0	1.00
loamy sand	38.0	16.0	8.0	80	2200.0	1.00
sandy loam	41.0	22.0	10.0	120	1200.0	1.00
loam	46.0	31.0	15.0	160	500.0	0.76
silt loam	46.0	33.0	13.0	200	575.0	0.80
silt	43.0	33.0	9.0	240	500.0	0.76
sandy clay loam	47.0	32.0	20.0	120	225.0	0.58
clay loam	50.0	39.0	23.0	160	125.0	0.47
silty clay loam	52.0	44.0	23.0	210	150.0	0.50
sandy clay	50.0	39.0	27.0	120	35.0	0.30
silty clay	54.0	50.0	32.0	180	100.0	0.43
clay	55.0	54.0	39.0	150	35.0	0.30

FIG 42 – Standard soil parameters (FAO)

Knowing these discrepancies the next step for this analysis was using another dataset for the soil parameters and check how well the results would correlate with the field data from the meteorological stations. The new soil parameter data has been taken from Hungarian research network (HUN-REN, 2024) and that dataset provided new soil parameters for the region, specifically for each of the points. To analyze as well how well the standard values that AquaCrop provides for Ksat for each of the different soil textures, two new simulations have been run for each of the sites. One while taking in consideration the USDA soil texture for each of the points and utilizing the standard values that AquaCrop provides for each texture and another utilizing the specific Ksat for each of the points.

Table 3 shows the difference in soil parameters from each of the different datasets for the surface layer.

Table 3 – soil parameters simulations

	Agrotopo					hungary soil					
Stations	**Texture**	**Ksat - Aquacrop**	**FC**	**SAT**	**WP**	**Texture**	**Ksat USDA -Aquacrop**	**FC**	**SAT**	**WP**	**Ksat**
apaj	loam	500	34	50	15	Loam	500	30.56642	42.21951	12.83411	6.6125398
borota	loam	500	33	48	14	Clay loam	125	25.54282	44.38335	13.35102	10.522793
csavoly	loam	500	35	48	14	sandy clay loam	150	30.0395	46.6776	14.5914	30.295965
csengele	sand	3000	31	49	13	clay	35	16.30338	41.53843	5.381576	49.259346
csolyopalos	sand	3000	30	48	12	clay	35	11.96997	42.89684	6.309484	187.44196
csongrad	sand	3000	31	49	13	Loam	500	28.89514	43.79094	13.62467	63.440269
fajsz	silt clay	100	35	47	17	sandy clay	35	36.99158	46.56603	19.59976	0.4444771
fulophaza	sand	3000	30	49	13	Loam	500	25.65304	41.81246	12.07318	19.975574
harta	loamy sand	2200	34	49	15	sandy clay loam	150	32.79635	45.60336	14.28027	5.2184701
hernad	sand	3000	30	50	12	clay	35	8.939511	41.03044	3.578464	90.556374
homokmegy	loam	500	33	49	15	sandy clay loam	150	31.00703	47.71582	18.20502	3.190614
izsak	sand	3000	28	48	12	clay	35	10.99911	41.38602	7.872583	258.32324
kalocsa	silt clay	100	35	48	16	sandy clay loam	150	31.96735	47.51631	19.54557	0.7486087
kecel	sand	3000	30	47	12	clay	35	11.33064	41.85612	5.75299	22.994823
kiskunfelegyhaza	loam	500	32	49	13	Loam	500	30.33614	44.91705	18.09769	10.143685
kiskunhalas	loamy sand	2200	33	49	14	Clay loam	125	15.60596	39.7766	8.181291	14.607512
kisszallas	loamy sand	2200	30	49	12	Clay loam	125	15.86756	40.8507	9.310092	25.518831
Kunszemtkilos	loam	500	31	50	14	Loam	500	26.02725	44.43876	12.55921	39.377037
kunpeszer	loam	500	33	50	14	Loam	500	27.59867	45.91656	14.15188	8.8669472
lajosmize	loamy sand	2200	30	50	12	Loam	500	17.64167	40.98136	6.852107	64.807022
Melykut	loamy sand	2200	32	48	14	Clay loam	125	10.81333	41.03601	7.304429	105.51717
Nagykiros	loam	500	32	50	14	Loam	500	16.97335	41.35119	7.642901	376.91357
Palmonostora	loam	500	34	49	15	Clay loam	125	24.29067	41.88156	13.96841	559.08112
Ruzsa	loamy sand	2200	30	48	12	clay	35	9.918707	39.406	5.196022	23.181309
Sandorfalva	sand	3000	34	49	15	Clay loam	125	13.13267	41.72457	8.218563	195.68369
Solt	loam	500	34	50	15	Clay loam	125	23.67883	45.11568	10.7722	27.07959
Sukosd	sand	3000	34	50	15	sandy clay loam	150	33.71981	46.98284	17.67896	1.0207294
Tazlar	sand	3000	30	48	12	clay	35	10.80107	43.06703	5.559392	160.22644
Varosfold	loam	500	33	49	14	Loam	500	26.36108	46.04242	14.91554	37.459206

From looking at table 3 it is possible to see that there is a big difference for some stations regarding the soil texture and soil parameters. This indicates that there will be different results when running the SpatialAquaCrop package. Another point to check is that the soil texture variation is lower in the Agrotopo soil data when compared to the new one from HUN-REN, 2024, this might indicate that the second dataset is more closely related to the reality on the field due to this texture variation.

So as mentioned before, two new simulations were done for each of the points, both utilising the FC, SAT and WP of the new dataset, but one utilizing the Ksat provided by the dataset and the other utilizing the texture provided by the new dataset and coupling this texture (USDA, 2024) to the Ksat values provided by AquaCrop (Fig 42). Results for some points can be seen bellow.

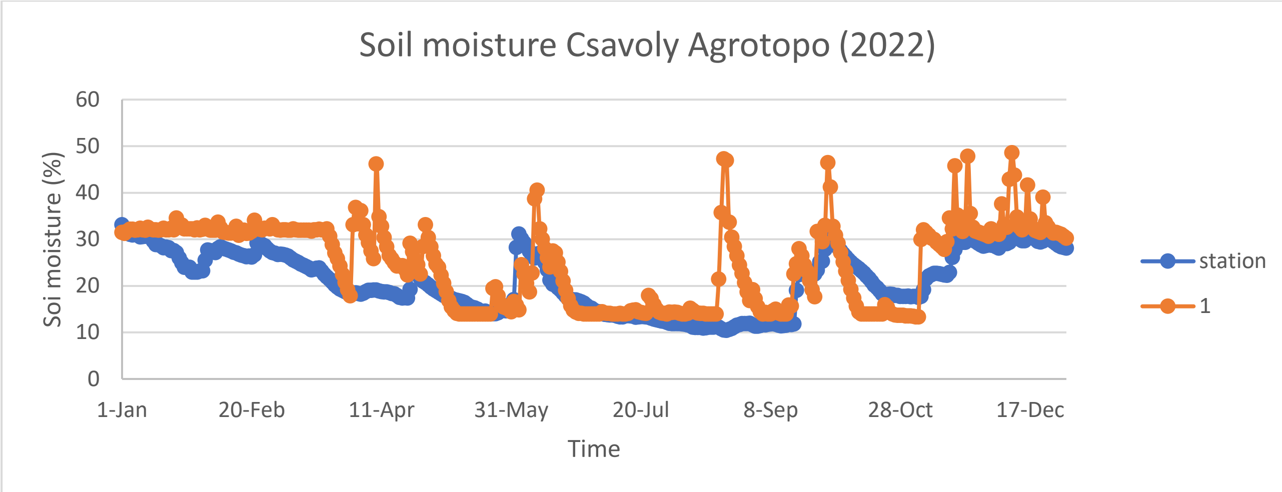


Figure 43 – Soil moisture Csavoly Agrotopo (2022)

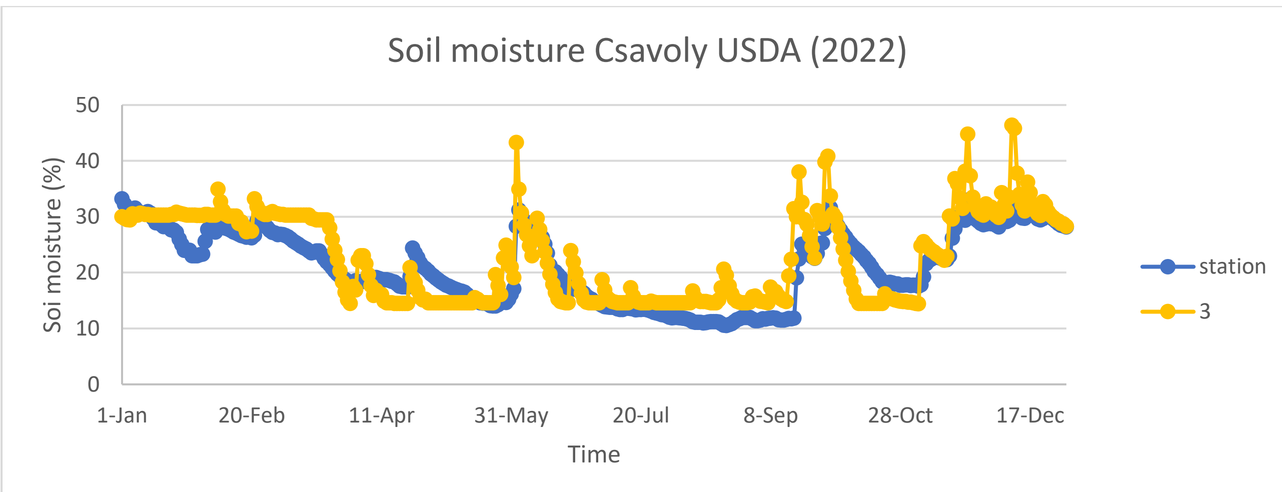


Figure 44 – Soil moisture Csavoly USDA (2022)

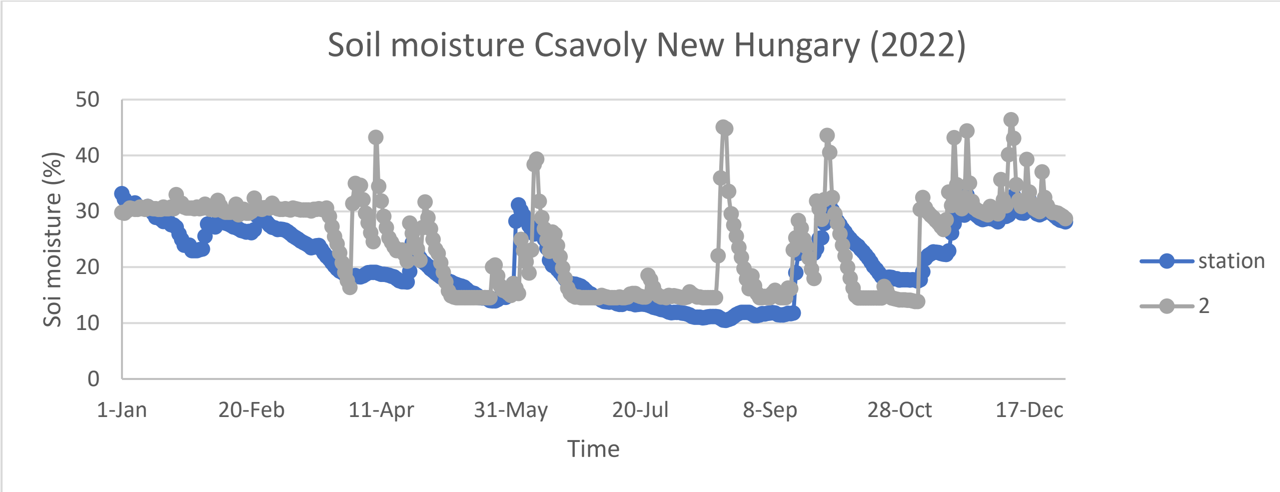


Figure 45 – Soil moisture Csavoly New Hungary (2022)

When looking at both figures 43 and 44 it is possible to see that there is a slight difference in the daily soil moisture variation, or in other words the degree in which this parameter varies daily due to how it is calculated in the model (raes et al., 2018). To check this variation the Pearson correlation for both timeseries was calculated for each of the simulations, with the Agrotopo one being 0.72, the USDA one 0.84 and the last of 0.71 (all then being statistically significant for having a p value lower than 0.05). The best correlation seen for this station was the USDA one and as we know that the main difference from the USDA simulation and the Hungary research network one was the Ksat, it is possible to assume that Ksat value highly interferes with the daily variation of soil moisture. Similar results can be seen for the point at the meteorological station in the region of Fajzs (figures 46, 47 and 48) which presented correlation values of 0.67, 0.81 and 0.55 respectively.

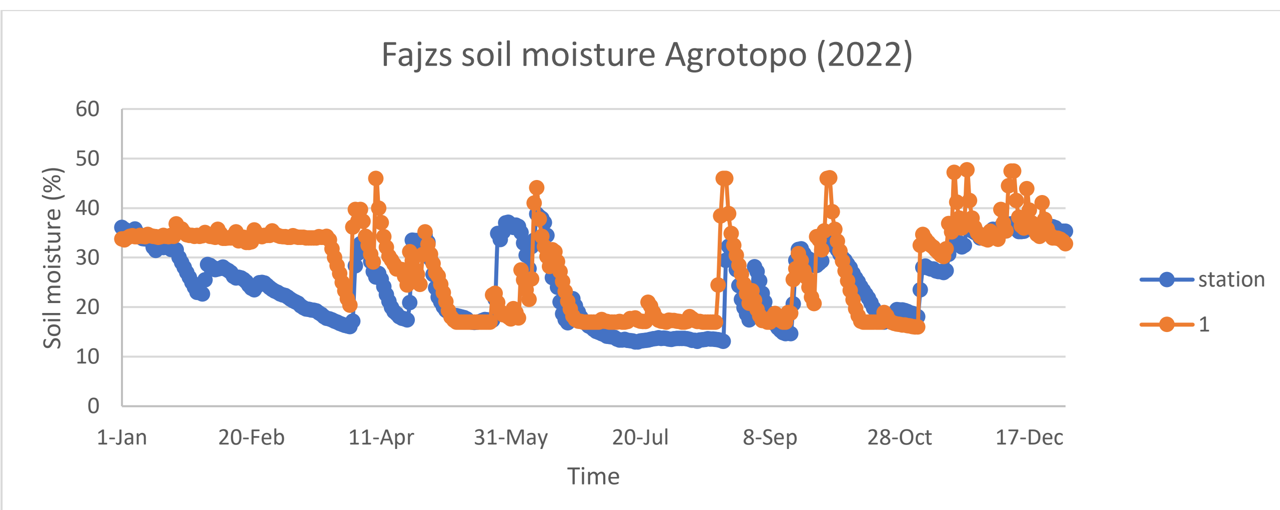


Figure 46 – Soil moisture Fajzs Agrotopo (2022)

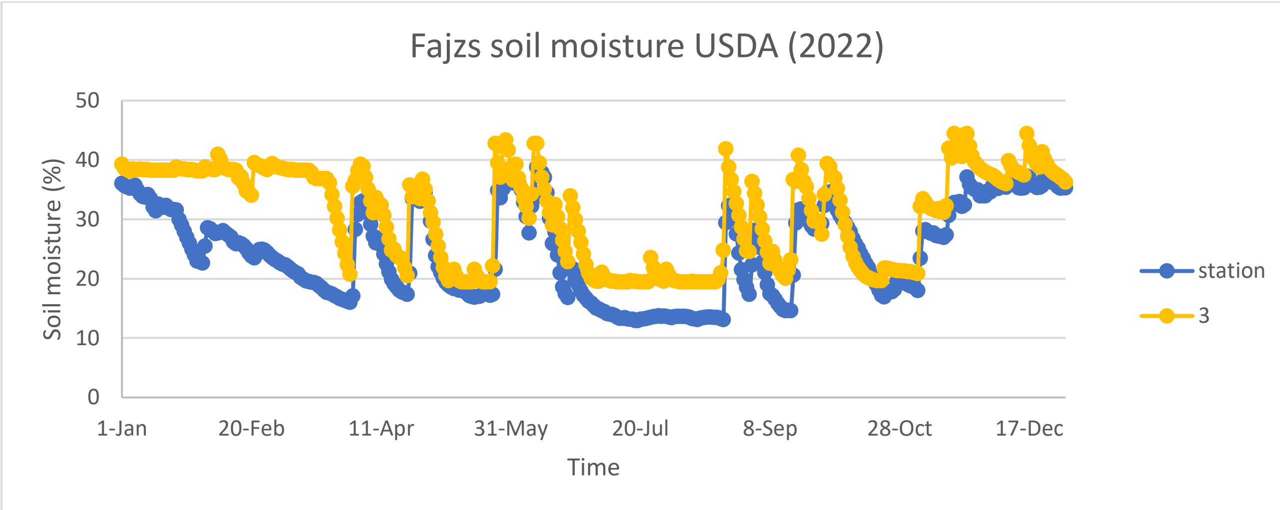


Figure 47 – Soil moisture Fajzs USDA (2022)

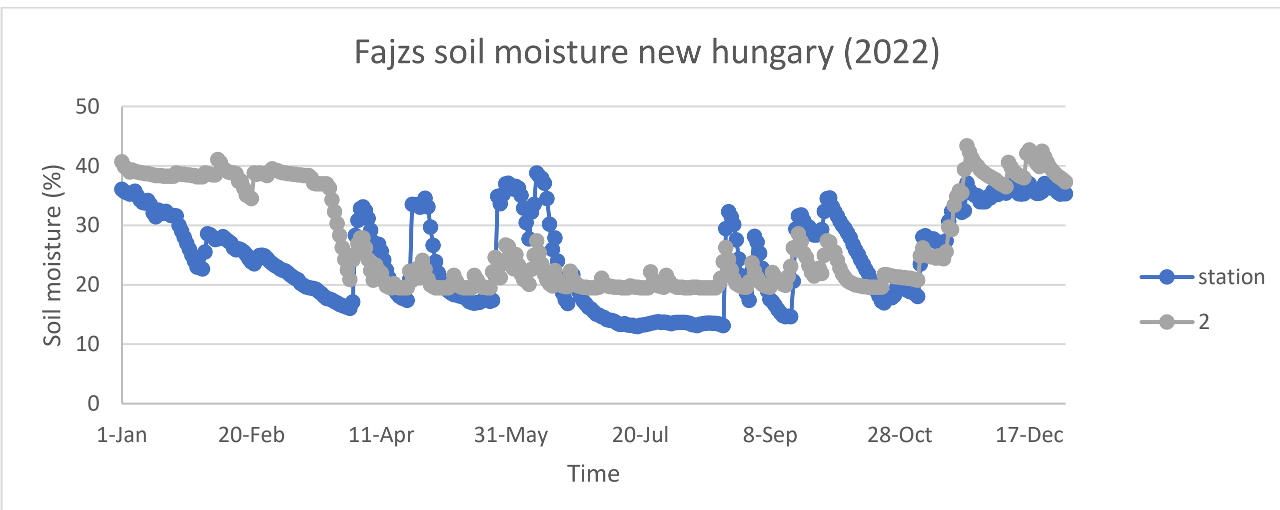


Figure 48 – Soil moisture Fajzs new hungary (2022)

Not all stations followed the same behaviour as these two prior ones, for example the one in Kunszentmiklós had its correlations respectively been (in accordance to figures 49, 50 and 51) 0.56, 0.69 and 0.73. So, in this station the simulation that got the best correlation was the one utilizing the Ksat from the Hungary research network dataset. Another detail that can be seen is that the difference in value from the soil moisture seen at the station to the modelled ones, even in the new hungary dataset which had the best correlation, has a bigger difference, when compared to the results of the prior stations. In this case it is possible to see that the WP is lower in the station timeseries than the simulated one, utilizing "soft calibration" and changing the WP to the lowest value that can be seen in the station timeseries a good difference can be seen (figure 52) and the correlation increased from 0.73 to 0.82.

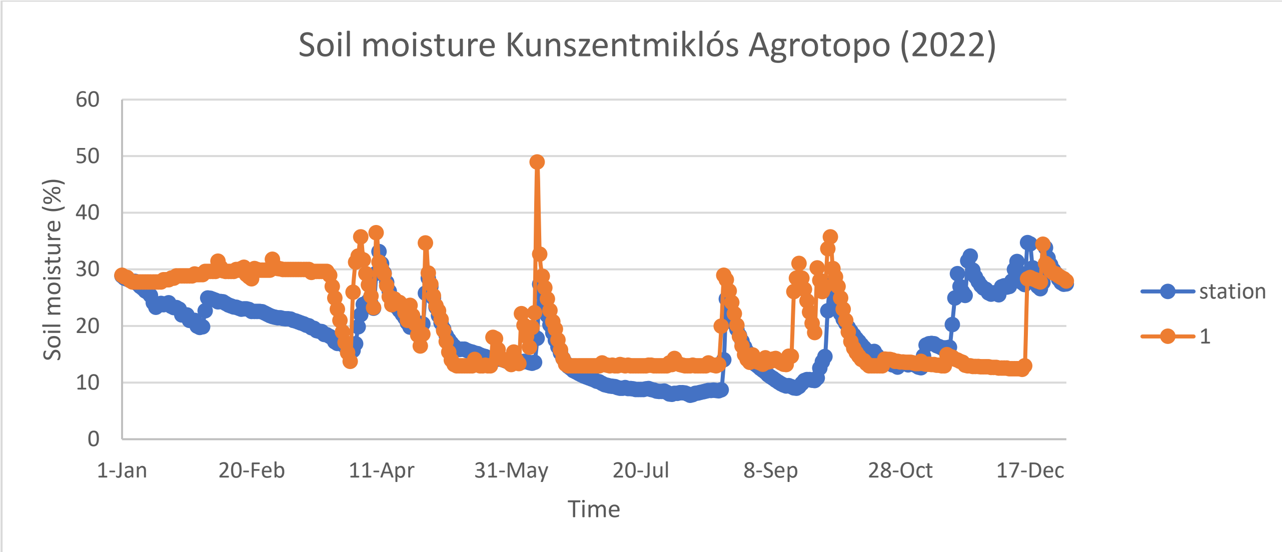


Figure 49 – Soil moisture Kunszentmiklós Agrotopo (2022)

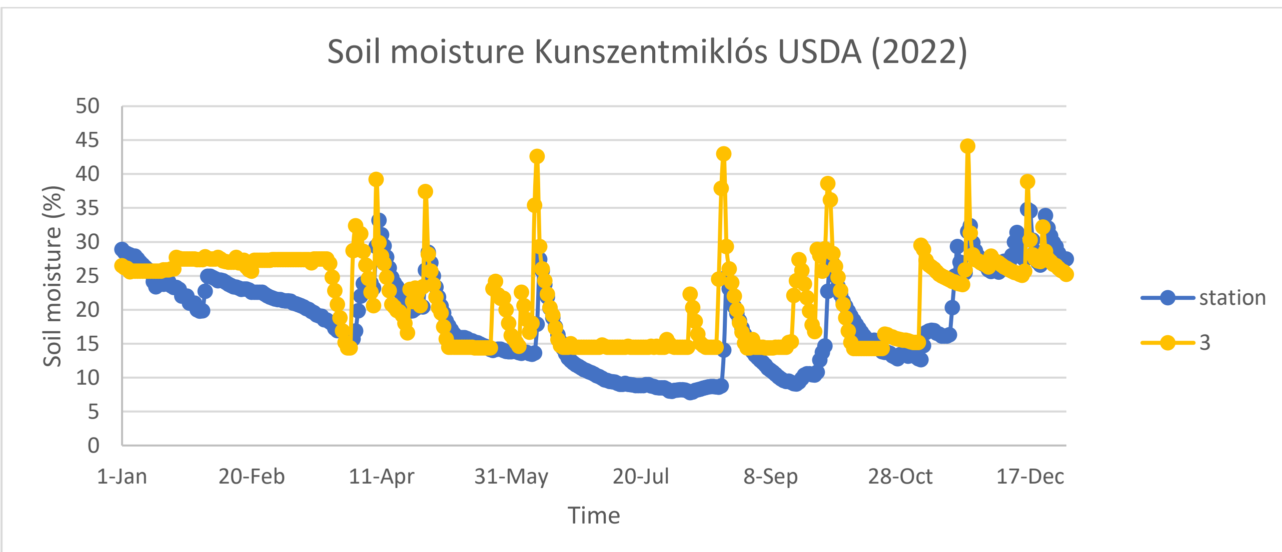


Figure 50 – Soil moisture Kunszentmiklós USDA (2022)

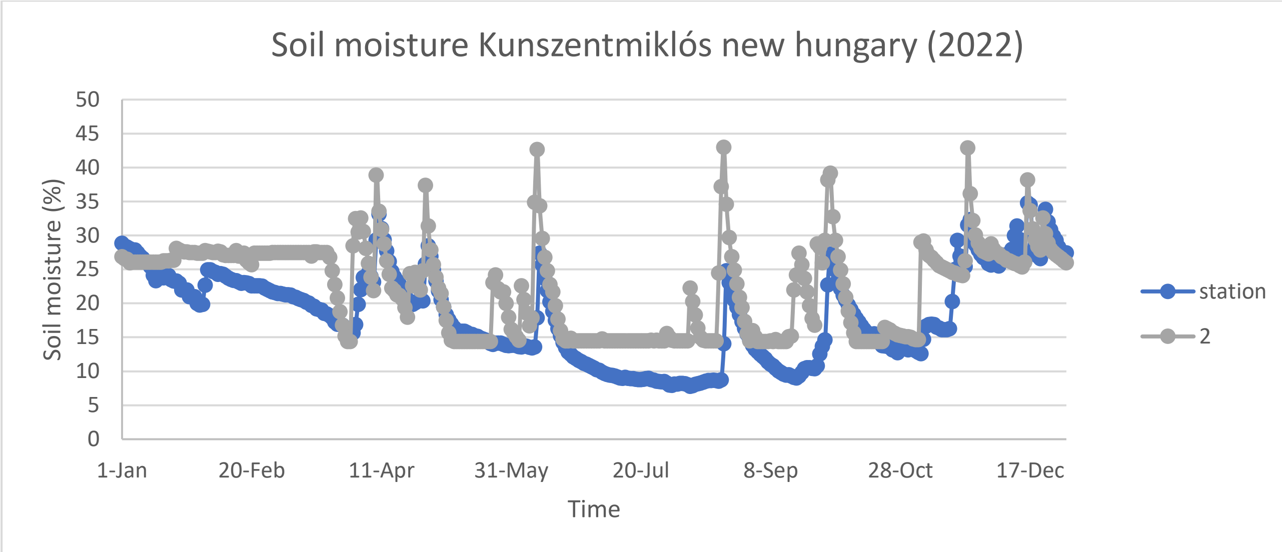


Figure 51 – Soil moisture Kunszentmiklós New Hungary (2022)

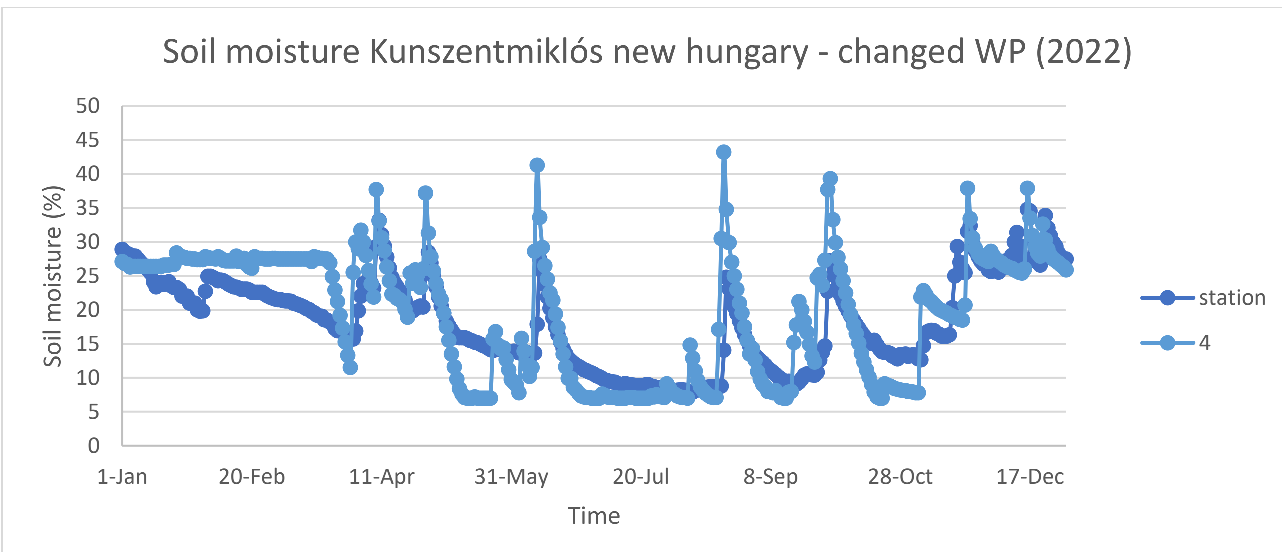


Figure 52 – Soil moisture Kunszentmiklós New Hungary – changed WP (2022)

In the case for this station the best lowering the wilting point was the best "soft calibration" that could be done for this station, but as it can be seen in figure 52 even though the overall correlation improved, but in some dates the difference got worse from before the change, for example around the month of May and October. Changing the Field capacity could as well improve the overall correlation and diminish the difference between the two timeseries.

Not all stations had their value improved/changed in a way that the correlation got higher than 0.7 (at least showing a small correlation), for these points (which an example can be seen for the station at Mélykút and Tázlár with figures 53, 54, 55, 56, 57 and 58, even after utilizing the three different simulation parameters no correlation could be seen between the different timeseries.

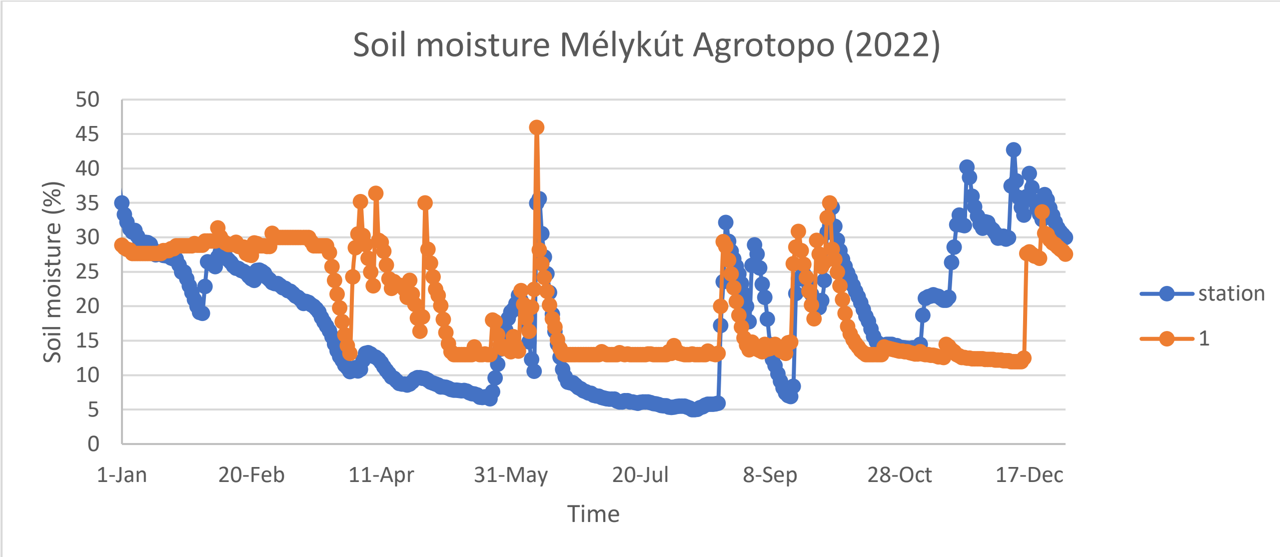


Figure 53 – Soil moisture Mélykút Agrotopo (2022)

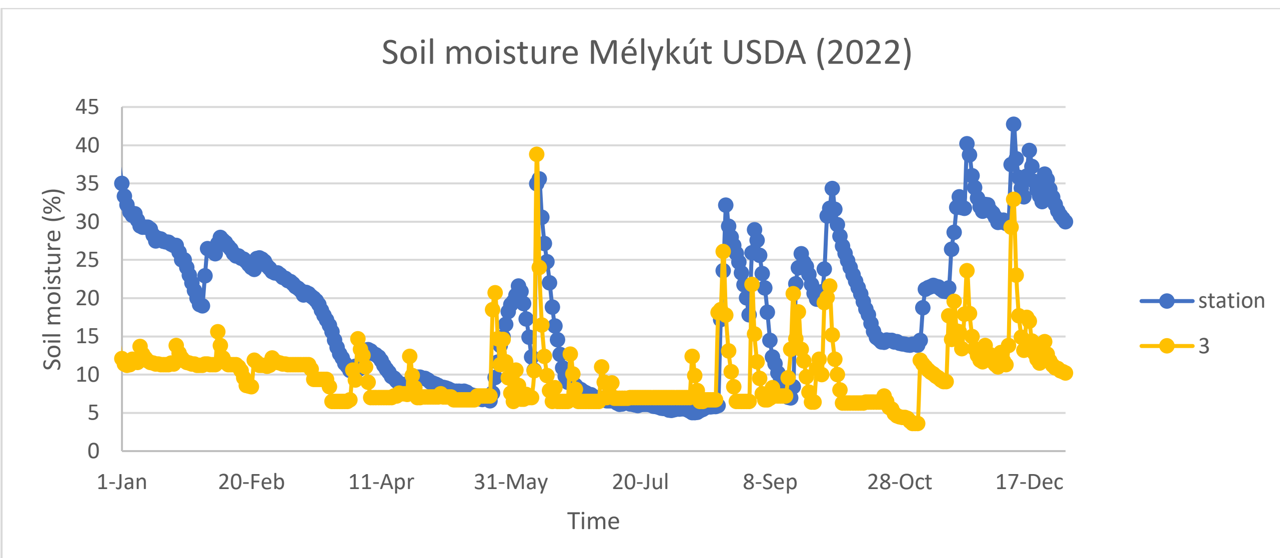


Figure 54 – Soil moisture Mélykút USDA (2022)

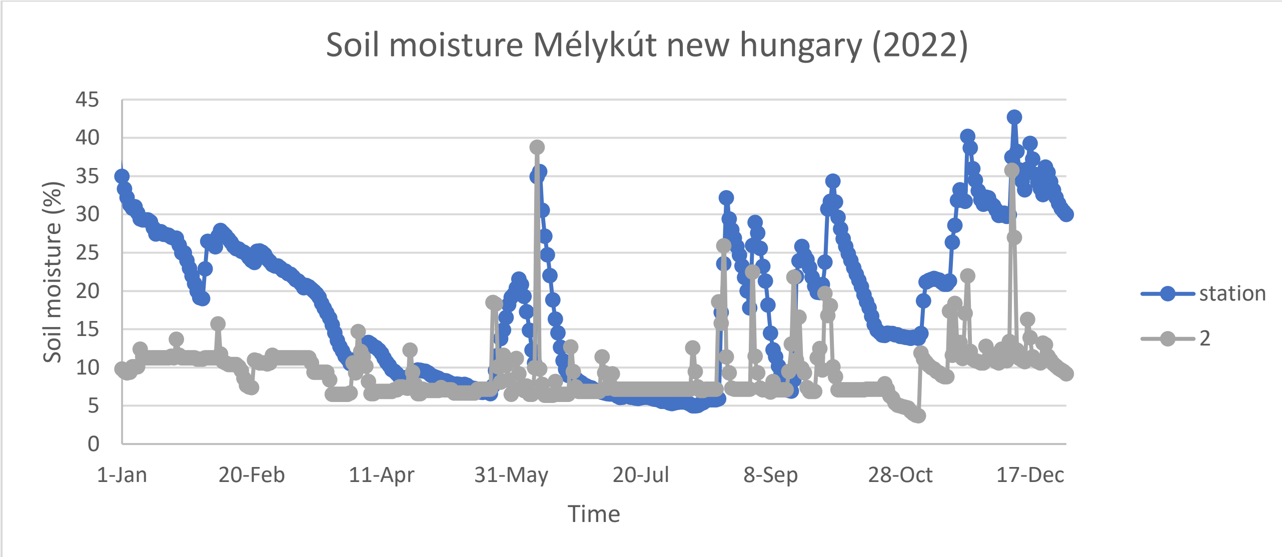


Figure 55 – Soil moisture Mélykút new hungary (2022)

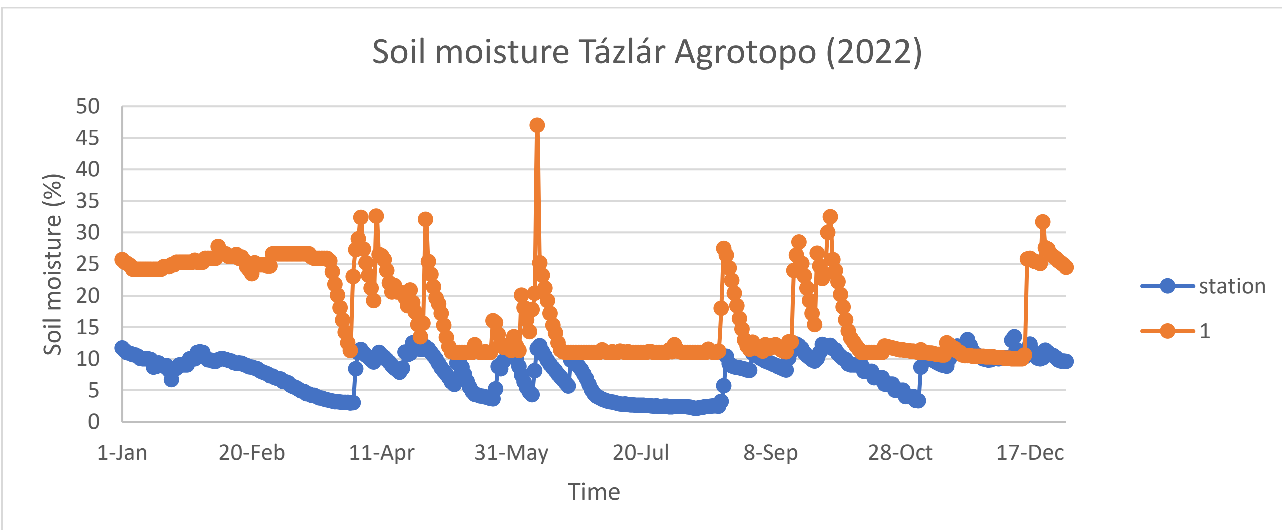


Figure 56 – Soil moisture Tázlár Agrotopo (2022)

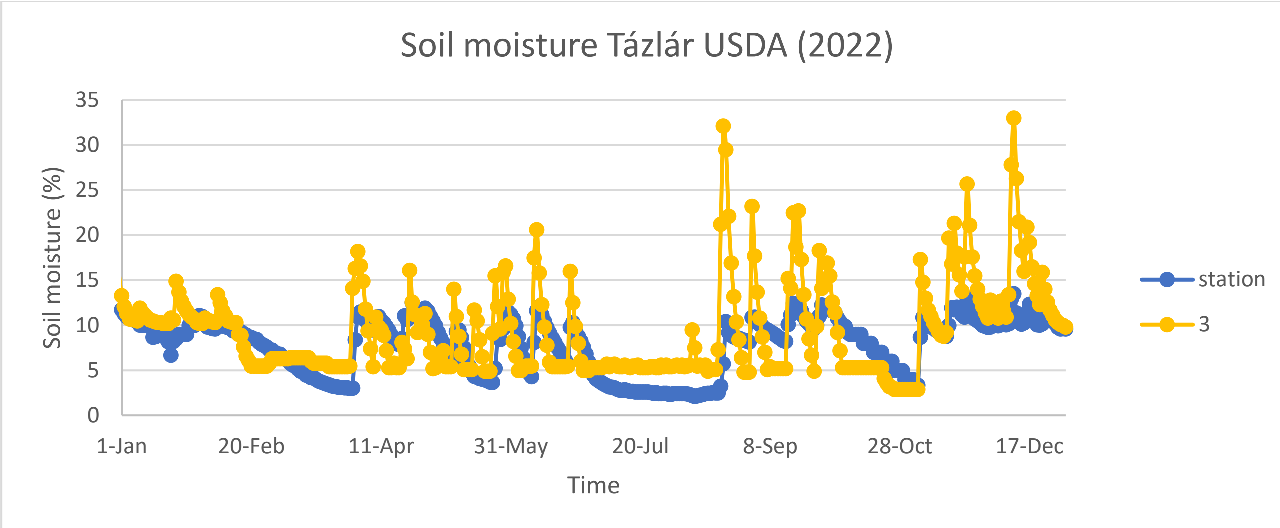


Figure 57 – Soil moisture Tázlár USDA (2022)

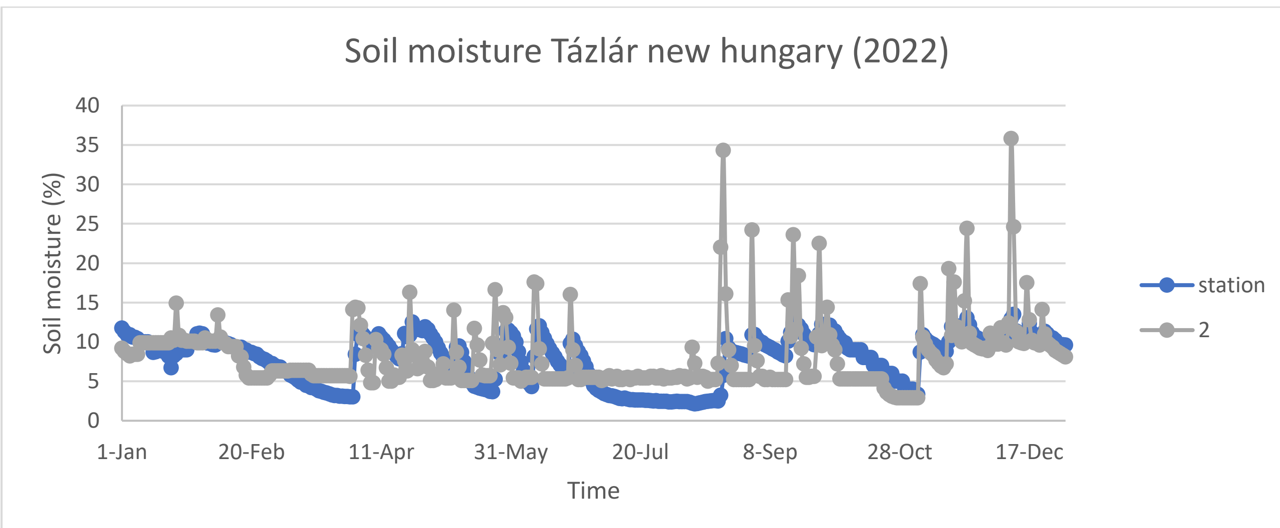


Figure 58 – Soil moisture Tázlár new hungary (2022)

Both of the stations of Mélykút and Tázlár show no good correlation in all 3 simulations, the highest correlation seen was for the USDA simulation for both stations with 0.6 and 0.59 respectively. As seen in table 4 most of the stations correlation improved with utilizing the new dataset so it can be assumed that this new dataset (HUN-REN, 2024) can represent the best the actual situation in the soil nearby these meteorological stations. So, for the stations that do not present a good correlation, a hypothesis can be made in which the soil around the station got disturbed from its natural state. This can have happened due to compacting of the soil or the soil around the station may have been disturbed during the station construction and not arranged back in a way that resembles the original soil in the region. This disturbance can be seen as well with the fact that for some of these points a quite big change in the soil field capacity and other soil parameters have to be made to achieve a good correlation between the different timeseries.

Table 4 shows all the difference in correlation for every different simulation for the points of this study case. As mentioned, before it can be seen an increase in correlation for most of the stations when utilizing the soil parameters for the Hungary research network and when changing just the Ksat for the standard values provided in AquaCrop as well.

Table 4 – Correlation values 2022 for all points

	Correlation (2022)		
Stations	**Agrotopo**	**USDA**	**HUN-REN, 2024**
Apaj	0.73	0.72	0.75
Borota	0.87	0.85	0.89
Csávoly	0.72	0.84	0.71
Csengele	0.47	0.77	0.47
Csólyopálos	0.60	0.76	0.66
Csongrád	0.47	0.58	0.57
Fajsz	0.67	0.81	0.55
Fülöpháza	0.61	0.76	0.78
Harta	0.78	0.85	0.85
Hernád	0.52	0.46	0.34
Homokmégy	0.42	0.76	0.51
Izsák	0.41	0.66	0.46
Kalocsa	0.6	0.67	0.71
Kecel	0.28	0.65	0.59
Kskunfélegyháza	0.41	0.71	0.73
Kiskunhalas	0.42	0.68	0.68
Kisszállás	0.48	0.53	0.53
Kunszemtkilós	0.66	0.74	0.73
Kunpeszér	0.56	0.69	0.73
Lajosmize	0.53	0.71	0.71
Mélykút	0.42	0.60	0.48
Nagykőrös	0.20	0.63	0.61
Pálmonostora	0.39	0.25	0.23
Ruzsa	0.31	0.64	0.56
Sándorfalva	0.25	0.65	0.52
Solt	0.63	0.75	0.75
Sükösd	0.46	0.78	0.87
Tázlár	0.34	0.59	0.44
Városföld	0.45	0.67	0.68

5.2. Study cases discussion

5.2.1 First case study discussion

SpatialAquaCrop was created with the aim to introduce an easier way to utilize the AquaCrop model (more specifically the AquaCrop plugin) to process spatial data in raster format and output the result from the AquaCrop model to a raster format as well, ensuring that the simulation runs without an issue and following the same idea of when the AquaCrop model was created, which was to facilitate and make more accessible its usage, and SpatialAquaCrop follows that philosophy by explaining to the user in an easy way how to use the different functions, if something is wrong and just expecting that the user give inputs on where the data is and which data will be used in the simulation.

The process of the package creation was only possible because of the different simulations that were done while the package was being developed as knowing what problems and necessities that users may encounter are essential for the development of the package and in the end resulted in a paper publication in a high impact journal (Barros et al., 2022). Even though there are other GIS applications for AquaCrop (AquaCrop GIS) and simulating the AquaCrop in another environment (AquaCropo), SpatialAquaCrop is a simpler approach for the usage of the AquaCrop model, as it uses the AquaCrop plugin for the model simulation, the difference is that SpatialAquaCrop provides a linear way to add the different inputs and different approaches for that (creating the text files manually or with the help of the AquaCrop software), besides that as the package was created in R, this environment provides easier way to analyze and process different types of data, specially raster datasets.

The first study case meant to show in a basic way how the package would function, if all the functions would be working and where some improvements could be made for the next versions of it. The results that can be seen in FIGS 15 until 20 show what was expected for this study case, a spatial variation based on the soil rasters that were used as input and some correlation between some of the different parameters, like infiltration and runoff.

As mentioned before at the state that the package was at the time of this case study, the only outputs that were available to output were the seasonal ones that AquaCrop plugin can provide, and these outputs were selected and they were properly showed as a raster, which was one of the main goals of this initial version of the package. The decision to rasterize the different input data was a successful one, because it made the package run the necessary functions without much processing delay, for example the run for the last function for the study area took around 7 to 10 minutes, being a reasonable time. Another good point for having all the data in a vector format is that if wanted, it is easy to anyone who has a small familiarity with R to select the necessary data needed and extract from any point in the package and save it in any format that R can transform it.

The results themselves from this study case, even though a simple one, show some relations with other results from prior studies, water footprint and yield (He et al., 2024,water footprint network, 2024). This is important as it means that the AquaCrop plugin was properly used but the SpatialAquaCrop package and the input data used was properly read by the package. Water Footprint is not something that AquaCrop model outputs but adding it to the package as an extra function for users to run seemed like a good decision, as calculating, green water footprint in this case, is quite relevant to modern studies for water management related to crop fields.

Even though not many new things were observed in this first study case, the main point of it was to have a proper first run of the SpatialAquaCrop package and check how well it performs and where some improvements could be made. One important point was to add outputs not just in a spatial manner but in a table format, which would facilitate the analysis of the results, another one was to add the daily results as well, not just the seasonal ones. These two features were added to the next version of the packaged and utilized for the next study case.

5.2.2 Second case study discussion

For the results of the second case study, we can start to see some similarities with the first study case. When looking at the results that the package provided for this grassland simulation, the seasonal results are in line with what is expected, as they show similar spatial variation and values like infiltration and runoff have a correlation with one another, which is expected, since both of those factors are dependent on the properties of the soil. Besides these two parameters it could be seen as well that biomass when compared to infiltration shows expected results when compared to the available literature (Meron et al., 2007), biomass and evapotranspiration show the same pattern, and this patter can be seen in literature as well (Tolk and Howell, 2009). All these relations between the different parameters really strengthens the credibility of the different input data that was used for this simulation, specially the crop parameters chosen for this simulation, as they are from a “crop” in which at the time AquaCrop did not support and did not have standard values for it.

As mentioned in this next version of the package, daily results are now available to be outputted, this being a great addition to the package, providing more options on how to analyse the results and which results that can be chosen to be analysed. Another advantage of the SpatialAquaCrop package is the potential generation of spatially distributed daily output data, which essentially allows the generation of “data cubes” for the specific study area, as demonstrated by figure 22. This opens the possibility of comparison and validation with earth observation data.

Comparison of daily time series output was done with data obtained from the monitoring station at the Gödöllő campus of the MATE university. The comparison reveals that while the application of the large scale (national) meteorological dataset is acceptable due to the close correlation of interpolated and measured precipitation data, there are potential limitations of using large scale (coarse resolution) soil information. However, as field-based or plot-based applications of the AquaCrop model would also inherently include similar potential sources of error (by not at all accounting for spatial heterogeneity), this is something that needs to be considered and addressed at the level of application.

Even though it is possible to say that large scale datasets can be accepted as input data, it is necessary to take in consideration the error that might come with it, specially for soil parameters, as the optimal would be always to get on site the necessary parameters, but the availability of large scale datasets from imagery methodologies give the availability of different analysis in areas with some field data scarcity.

One of the more apparent differences between simulated and modeled daily data is for soil moisture, as they don’t act at the same way throughout the time series. Figure 23 shows clearly that some of the peak values before October are the same, because of the similarity between the precipitation data, even though between those peaks the field data shows more variability than the modeled one.

What is different between the soil moistures of the measured and the simulated cases is that after the middle of October the values from the monitoring station stabilize, or in other words the soil gets saturated, while the modelled one starts to decrease. This phenomenon can be explained in the model by the decrease of the canopy cover of the grassland, the lower average temperatures and decrease in precipitation (Figure 24), making the soil moisture decrease, and a superposing all these factors. For the soil moisture values from the monitoring station the opposite happens, as the soil becomes saturated and stays with a similar value for the rest of the time series. After this study case has been finalized a more in-depth check has been done for the soil moisture results seen for the winter period for the meteorological station, and it has been noticed that during winter soil moisture values could not be considered as there was some interference happening.

Beside this bigger difference, it can be seen that the precipitation has an effect in the soil moisture (Figures 25), especially in the upper layer of the soil (0,1 m), where the changes in soil moisture are more visible.

While the above differences in modeled and measured soil moisture dynamics are significant, it is important to note that limitations of input data can clearly be the source of such errors. The differences are clearly driven by soil parameters, most of which used in this study have been derived from a 250 by 250m raster dataset that has been designed at a European level. This can clearly be the source of such errors and highlights the importance of scale and resolution. However, in this scenario (also limited by the applied model), the effects of topography and surface conditions (such as ruggedness) have not been considered. But according to Vereecken et al. this approach can have benefits, too, since the very detailed local parameters are usually not representative enough for the whole modeled environment. This issue with soil parameters dictating the error for the simulation is addressed in the last study case, as it is one of the main points observed in that study case.

The difference from what the first version of SpatiaAquaCrop to the version used in this study case can output is quite apparent, and with a wider and better choices for output and their format, daily/seasonal outputs in table format or daily/seasonal outputs in a spatial format. This enhances the quality of how the outputs can be analyzed, in this way improving the quality of any research that would utilize this package as a methodology.

5.2.3 Third case study discussion

When comparing both of the results for AquaCrop and Hydrus that can be seen in figure 29 and 30, as mentioned AquaCrop shows a higher daily variation for the soil moisture results. Even when taking in consideration all the errors of the input data that were found after this short analysis was done, the importance of it still remains, as it can be seen a difference for both models' soil moisture results. The idea of utilizing another model to verify how well their outputs are when comparing to each other is to have a broader view of different methodologies. When taking in consideration different references the Hydrus model does present as an alternative for simulating soil moisture and it could be utilized together with AquaCrop for developing a methodology that would bring the best for bother models. But for this study that avenue was not chosen, as the development and usage of the SpatialAquaCrop package has been the aim of this PhD study, learning and focusing on another model would not be beneficial for this study in specific, but this small study led to some good ideas for some different methodologies, which were presented in the soil conference in 2022.

5.2.4 Fourth case study discussion

The last stable version of the SpatialAquaCrop was developed for this study case, as it improved how smoothly the data is read and processed. As this study case was separated in two parts, one for the Martonvásár area, soil moisture comparison on a maize field, and one for the experimental field of the MATE university in Gödöllő, NDVI comparison between modeled biomass and green canopy cover, both of these are point based validations, so part of the input data was not obtained from raster files. Even if that is the case it has been pertinent to keep using the SpatialAquaCrop package, as the different points can be run in a "batch processing way", without the need to reset the simulation for each point. This way has been possible with the package due to some manual change of how the input data was introduced in the .CSV files that the package uses to get the data, besides that no change was done in the different scripts of the package.

When evaluating the soil moisture for maize in 2020 at Martonvásár (Figure 35), it is possible to see some trends between both of the timeseries and significant and good correlation coefficient between them both. For the beginning of the timeseries they showed around a difference between both of the timeseries of 7%, but that value decreases as two "significant" precipitation events that occurred, one on May 24th and the other one in June 12th. It is interesting to see that the values tend to get closer after the precipitation events and another important point to take into consideration is how the AquaCrop model reacts faster to the rain in relation to what happens in reality in the field. This can be explained due to how AquaCrop calculates soil moisture (de Roos et al., 2021) and how it doesn't take in consideration some soil characteristics that would "smoothen" this rise in soil moisture due to the precipitation. As the soil parameters for this comparison were taken from the work of Sándor (Sándor et al., 2020) we can exclude that this different from both timeseries comes from some difference in the soil parameters at the area.

One good conclusion that can be taken from this comparison is that the model works in a good manner when compared to data that was collected in the field, when comparing to the spatial data that was used for prior study cases, adding more to the many different model validations that were done before (de Roos et al., 2021; Tsakmakis et al., 2018;, Dalla Marta et al., 2019). This difference will be analyzed better in the next, and last, study case of this PhD thesis, as utilizing raster datasets is one of the main goals of the methodology developed in this thesis.

When analyzing figures 32, 33 and 34 and later their corresponding correlation values it can be seen that there is a good correlation between modeled biomass and NDVI until the senescence period of winter wheat for this region in Hungary. It has been seen that this correlation can be seen with other crops as well in other different regions, but they might be region dependent (Abi Saab et al., 2021; Tenreiro et al., 2021). Despite this it is possible to say that AquaCrop can give good results for the modeled biomass as they correlate quite well with NDVI that was seen in the studied area.

As for green canopy crop cover the R^2 values were lower than biomass while considering a linear regression model but showed better results when considering a polynomial model of second order.

When taking into consideration CC values over 80% an exponential regression model became a better fit and that can be seen better for the 2021 analysis, because there were more points that could be used for the comparison in relation to 2020. It is interesting to note that this exponential behavior starts to happen when CC is around 80%, which is close to when the model considers that crop reached its maximum rooting depth (parameters were established from winter wheat crop reference (Szasz, 1988).

Even though these correlations between biomass and CC with NDVI could be found for winter wheat in our chosen region in Hungary, this could change for other regions of the country, also depending on winter wheat varieties. Different studies support that NDVI and CC have a correlation for different crops, even for winter wheat as well (Tenreiro et al., 2021, Lykhovyd et al., 2022). This supports even more the data that shows this correlation for these two parameters. The same can be said for biomass and NVDI (Goswami et al., 2015; Farias et al., 2023).

An advantage of the applied methodology is the potential generation of spatially distributed daily output data, which essentially allows the generation of "data cubes" for the specific study area. This opens the possibility of comparison and validation with earth observation data, as well as for related agronomical applications, such as irrigation scheduling.

5.2.4 Fifth case study discussion

For this last study case of this PhD one important point is the availability of different soil datasets (table 3), for comparison, as some discrepancies due to, most likely, soil parameters in the past study cases have been seen. Even though both of these datasets have been obtained from interpolated data, it is possible to see from the results of the comparison of soil moisture, that the dataset from the Hungarian research network has shown better results than the one from Corine. As this comparison was done for the south region of Hungary it is not possible to say that for sure the Hungarian research network is more accurate than the other one in general, but for these points and region these parameters show better results when simulating soil moisture.

Besides the soil parameters, another point in which can be compared with prior study cases is the crop used in the simulation. As in the second study case a grassland simulation was attempted, in this last one grass was simulated as well utilizing AquaCrop. Even though AquaCrop is not first meant to simulate grass it has been possible as seen in different studies (Kim and Kaluarachchi, 2015; Allan et al., 1998; Terán-Chaves et al., 2022). The new grass crop that was created utilizing these studies in mind is not meant to completely follow reality but to try to create a grass crop which would always be present on the soil surface and mimic the water consumption/root depth and plant growth from the real grassy crops. As seen in Figure 36 the first year of the 3 year simulation showed a "build up" period for the simulated soil moisture, that is thought to be mainly a cause of the crop parameters, as the "new crop" has been designed to be and stay mature as fast as possible, but there might have been some issues with the different parameters used in the crop file, which may have caused this "build up" in the first year. For the second and third year it is possible to see that the soil moisture started behaving more accordingly to what is expected and because of that only the third year has been used for comparison.

As the main goal of this study case was the comparison of soil moisture from the simulated data and the on site data from the meteorological stations and that this soil moisture data from these stations may represent a base soil moisture value for the region, as the area whether the soil moisture has been assessed near the stations are most likely covered with grass. This base soil moisture is important as it shows a value of soil moisture that may be expected in the region and some different thresholds for when low infiltration or high runoff is to be expected (Yu et al., 2023).

What has been seen on the different comparisons is that the different points show different rates of correlation between the simulated datasets and the on site soil moisture. And that changing the soil moisture parameters change the correlation value. This aspect let to believe that some points in the raster datasets dot not really represent the parameters seen on the field. This shows that there has a change in which the soil in some of these stations may have been tempered, possible being affected by compaction or added organic matter in the soil, these affect on the value for Ksat and field capacity (Lebert et al., 2007; Seehusen et al., 2019; Minasny and McBratney, 2017). Of course it is impossible to know for sure if these effects are actually happening in reality, but as two different soil parameters sets were used in this study (and the one from the Hungarian research network seems to be an improvement to the Corine one) it can be said that it is expected that the best results from then would properly simulate the soil parameters in the region. So, considering that the best correlation results represent soil parameters that match with reality, and that has happened for most of the points (table 4), so the points which do not show this good correlation can be considered to have something that changes the soil characteristics.

When looking at the results from the 3 different runs it is possible to see that when utilizing the soil parameters from the Hungarian research network the correlation results were generally better and showed a small or big correlation, higher than 0.7. And utilizing the Ksat from AquaCrop in correlation to the USDA texture the number of stations which show a good correlation increase. These variations in soil parameters are important for when analyzing the results from the AquaCrop model, as they show how different parameters, soil moisture in this case, are affected by the increase or decrease of a specific parameter. A parameter that made a big different in the correlation value has been the Ksat, as it mainly changed how the daily variation of soil moisture behaved.

This study case showed a more point based approach when in comparison to the other studies, as the other ones have already set the spatial capabilities with the methodology of utilizing the SpatiaAquaCrop package. So in this last study a point based approach was chosen, with a focus on the soil parameters modeling and how they affect the overall results of the AquaCrop model, and more specifically soil moisture. Besides showing how the soil parameters affected the soil moisture results, it showed as well the importance of the quality of input data, as there is a significant difference from both soil parameter datasets that were used in this study.

6. CONCLUSION AND RECOMMENDATIONS

Nowadays, given the increasing amount of available spatial and remotely sensed data, combined with the need of agricultural water management, an increased number of applications would require raster-based utilization of AquaCrop. The purpose of this PhD was to develop such a methodology. In data scarce regions where accurate yield and soil moisture measurements are not available we can utilize remote sensing based and also model based estimations.

The SpatialAquaCrop package was made in a way that it would give an easy and understandable option to utilize the AquaCrop model not just for a specific point but rather to an area (utilizing raster based inputs). In its current state the package can output all the outputs that the stand alone version of AquaCrop is capable to and besides this the package has a function to output the green water footprint. As shown in the different study cases the package has show the versatility and capability to properly run the AquaCrop-plugin and prepare all the input data that are necessary for the simulation. The advantage of being able to read and output data in a raster format or in different tables for the daily results is a great advantage, as it opens more advantages for the utilization of the AquaCrop model, instead of the point base software.

When seeing the results from the five different study cases from an overall viewpoint, one thing that stands out is the importance of input data to the outputs the AquaCrop model can give. Study cases 1 and 2 showed different correlations with different outputs, which had similar trends to what has been seen in some prior studies, and one important was that it was possible to simulate grass with not big errors. Study case 4 showed that it is possible to correlate and utilize satellite base data for input and correlation to the model results with good results. That is important as in areas with data scarcity it is possible to utilize satellite based data to make up for missing data. Study case 5 mainly addressed one point that was becoming apparent in the prior cases, which was the quality of the input data, as that could be seen that the HUN-REN soil dataset gave better results when compared to the CORINE dataset. As the Corine dataset has been used to all other studies, this shows that maybe utilizing this new dataset to prior studies might improve past results, especially when utilizing Ksat from the standard table that AquaCrop provides. One important thing to highlight is that with the new soil dataset that OVF has released recently it could open new possibilities for the analysis of the region of study case number 5, as now there is a detailed soil description and data for each of the different meteorological stations, which now can provide data for validating the modeled results, but due to the time this dataset has been released, validation would be done in a future research.

When taking in consideration the different results and the practical applicability of this methodology, one possibility which could be approached is utilizing it together with different climate prediction models, so in this case this methodology could be used to predict, for example, floods, necessity of irrigation for a particular period, general soil water content and other environmental characteristics which would be pertinent for the applied data.

Most of this research was done inside R environment where the package was created, which enhances the possibility of an easier way for analysing and utilizing the different outputs that SpatialAquaCrop provides. Also, if the user has some programing knowledge in R, it is possible to add additional outputs to the package if necessary.

7. NEW SCIENTIFIC RESULTS

1. I have successfully developed an R-based methodology and package (SpatialAquaCrop) for the raster-based implementation of the AquaCrop model, demonstrating that the model can be utilized to generate spatially explicit predictions where data is available.
2. I have demonstrated that the methodology is suitable for generating not only seasonal estimates, but also daily grid outputs of selected parameters, making it suitable for further research into drought management and irrigation applications.
3. I have demonstrated that the estimated biomass and green canopy cover values of AquaCrop (utilized with the SpatialAquaCrop package) correlated well with Sentinel-1 based NDVI values in case of winter wheat, proving that the developed methodology could be particularly useful for applications combined with remote sensing.
4. I have demonstrated that with the available data for Martonvásár 2020, under winter wheat, AquaCrop has systematically produced higher estimates of volumetric soil moisture content than the measured values.
5. I have developed a methodology to apply AquaCrop for selected points of the Hungarian National Drought Monitoring Network, and demonstrated that there are notable differences in the accuracy of the estimates, that can be most likely be associated with inaccurate soil data parameters, derived from spatial datasets. This indicates that spatial extension of the soil moisture data will likely carry similar limitations.
6. I have demonstrated that the utilization of the new HunSoilHydroGrids dataset has significantly improved the estimates of soil moisture, making this dataset more feasible for generating spatial estimates of soil moisture.

8. SUMMARY

Thesis title: Spatial AquaCrop. A new tool for utilizing AquaCrop in a raster based environment

Author: Vinicius Deganutti de Barros

Course: PhD Evironmental Science

Institute: Institute of Environmental Sciences

Advisor: István Waltner

Water has been a key resource for many areas in human society, specially for agriculture, in which water is a limiting resource and at the same time agriculture is one of the biggest utilizers of water. For that Water management is a key point for agriculture and there are many ways for that, one in specifically is crop models, which can give different information on how to properly manage crops, specially for needed irrigation. One of these models is AquaCrop, which has been created by FAO with an intent to simplify crop modeling and SpatialAquaCrop is a package that has been developed in this PhD to utilize the AquaCrop model in a raster environment and not just as a point based simulation. This PhD objective is to show the SpatialAquaCrop package and its efficacy and for that five different study cases have been done during the length of this PhD. The studies mainly focused on validating soil moisture with data observed on the field, correlation of different simulation outputs with one another and with other parameters, such as green canopy cover with NDVI, and in the end analyzing the efficacy of different soil input data and how this data can affect on how the AquaCrop results are simulated. With the results from these study cases it could be seen that the package has worked and proved quite efficient in outputting the necessary data in a raster format or in daily output in a table format when needed. The study opened new points for new studies, such as upgrading the package with newer and different tools, further access the quality of two different soil data sets for Hungary.

9. AKNNOWLEDGEMENT

First, I would like to thank my supervisor Professor Waltner István, as without him this would never have been possible, and I would like to emphasize how important of a role of supervisor and friend he has been for me for the time of this research.

I would like to thank my family in Brazil and my family that I have gained by the end of this PHD, without their help and support I would never be able to complete this research and be able to properly defend it, mainly the support that my Wife Ayaka has been giving me since we are together and lately the everyday smiles that I can see from our son, all of that was necessary for this to be finished.

Besides that I would like to thank all the staff of Mate university who helped me during these years and specially by the end of the research. As well I would like to thank all the university colleagues who I worked together and because of them a lot of results were obtained for this research.

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