Karst spring discharge modeling based on deep learning using spatially distributed input data

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Abstract. Despite many existing approaches, modeling karst water resources remains challenging ~~and often requires solid~~ as conventional approaches usually heavily rely on distinct system knowledge. Artificial ~~Neural Network approaches offer a convenient solution by establishing a simple~~ neural networks (ANN), however, require only little prior knowledge to automatically establish an input-output relationship~~on their own. However, in this context, temporal and especially~~. For ANN modeling in karst, the temporal and spatial data availability is often an important constraint, as usually no or few climate stations ~~within a karst spring catchment are available. Hence~~are located within or near karst spring catchments. Hence, spatial coverage is often ~~unsatisfying and can introduce severe uncertainties~~ not satisfactory and can result in substantial uncertainties about the true conditions in the catchment, leading to lower model performance. To overcome these problems, we ~~use 2D-Convolutional Neural Networks~~ apply convolutional neural networks (CNN) to ~~directly process gridded meteorological data followed by a 1D-CNN to perform~~ simulate karst spring discharge ~~simulation~~and to directly learn from spatially distributed climate input data (combined 2D-1D-CNN). We investigate three karst spring catchments in the Alpine and Mediterranean region with different ~~meteorologic-hydrological~~ meteorological-hydrological characteristics and hydrodynamic system properties. We compare ~~our 2D-models~~ the proposed approach both to existing modeling studies in these regions and to own ~~1D-models~~1D-CNN models that are conventionally ~~based on~~ trained with climate station input data. Our results show that ~~our~~all models are excellently suited to model karst spring discharge ~~and rival~~ (NSE: 0.73-0.87, KGE: 0.63-0.86) and can compete with the simulation results of existing approaches in the respective areas. The 2D-models show a better fit than the 1D-models in two of three cases ~~, learn relevant parts~~and automatically learn to focus on the relevant areas of the input ~~data themselves and by~~ domain. By performing a spatial input sensitivity analysis, we can further show their usefulness to localize the position of karst catchments.

1 Introduction

Karst aquifers and karst springs are crucial for freshwater supply in many regions and 9% of the global population partly or fully rely on karst water resources (Stevanović, 2019). Karst systems in general are characterized by high structural het-

erogeneity due to the at least in large parts unknown conduit network, which controls the highly variable groundwater flow. These factors make modeling difficult, nevertheless different approaches exist, which Jeannin et al. (2021) classify as hydrological models (fully distributed models), pipe flow models (semi-distributed models), and data-driven models (including reservoir models). Artificial neural networks (ANN) or its subgroup of deep learning (DL) models are part of the last group. In contrast to the other two categories, which usually require detailed system knowledge in order to achieve high quality results, DL approaches offer an alternative possibility of modeling, by being able to establish an input-output relationship automatically, without detailed system knowledge necessary. Even though ANNs are not a standard method in karst modeling yet, different types of ANNs have been applied in modeling karst water resources for quite a long time. As one of the first applications Johannet et al. (1994) showed that karst spring discharge modeling is possible with ANNs. Since then, application of ANNs in hydrology in general received ever growing research attention (e.g. Maier and Dandy, 2000; Maier et al., 2010). This has amplified even more in the last years, mainly because of the recent success of DL models (e.g. Kratzert et al., 2018). Rajaee et al. (2019) more recently reviewed applications of ANNs on groundwater; Sit et al. (2020) summarize applications on hydrology and water resources in general. Recurrent neural networks (RNN), such as long short-term memory (LSTM) (Hochreiter and Schmidhuber, 1997) are standard models for time series modeling, because they possess explicit or implicit memory to remember past time steps, which helps to infer the future. A consequence is that they are trained sequentially, which can make them computationally expensive. Convolutional neural networks (CNN) (LeCun et al., 2015) on the other hand use convolutions along the time axis (1D-CNNs) to learn temporal features and can be trained batch-wise, which therefore usually makes them computationally favorable over RNNs. One example for this fact exists in the related domain of groundwater level forecasting, where Wunsch et al. (2021) showed that 1D-CNNs are considerably faster than RNNs in the case of single site model application. CNNs at the same time exhibited more stable results through less dependency on the random network initialization and achieved some of the highest performances in this specific study (better than LSTM). Other authors similarly applied CNNs successfully for either groundwater level forecasting (Afzaal et al., 2020; Lähivaara et al., 2019; Müller et al., 2020) or rainfall-runoff modeling (Van et al., 2020; Hussain et al., 2020). Müller et al. (2020) find in contrast to Wunsch et al. (2021) that CNNs take a considerably longer time to optimize than LSTMs, yet both studies agree, that they outperform LSTMs in terms of accuracy. Given these favorable properties of CNNs, we choose 1D-CNNs for karst spring discharge modeling for our study. To our best knowledge

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Jeannin et al. (2021) is the only study yet, applying CNNs for karst spring discharge modeling in some first experiments and they also find CNNs to be superior over LSTMs in terms of testing performance. ~~Especially in direct comparison to concept based modeling, where shorter time series can be sufficient to achieve satisfying modeling results, one~~ Data-driven approaches in general are considered to be black boxes. A way to still build confidence in a model's decisions is to understand what the model is doing (ideally, even why) by using explainable artificial intelligence (XAI). There are different approaches, which are potentially suited for this purpose, depending on the specific goal. Such approaches not only are useful to gain trust, but also help during model building to debug the model and to check what aspects it is focusing on (McGovern et al., 2019). The class of wrapper methods (Kohavi and John, 1997) incorporates both the data and the trained model to interpret what a model has learned. Methods from this class are for example impurity importance for determining feature importance in random forest (RF) models (Louppe et al., 2013), permutation importance (Breiman, 2001) both for RF and DL models, and partial dependence plots (Friedman, 2001) that also reveal why a predictor is important. See McGovern et al. (2019) for an overview on these and several other model interpretation and visualization methods. Especially for image alike data, input sensitivity approaches seem suitable, as focus regions of the model on the image can be visualized. Two well known approaches are occlusion sensitivity (Zeiler and Fergus, 2014) and RISE (Randomized Input Sampling for Explanation) (Petsiuk et al., 2018). Both methods show how relevant each pixel or area is for the decision of the model (image classification) and can generate an importance heatmap (saliency map) for visualization. The idea behind both algorithms is to use masked versions of an input image and by obtaining the respective model output to learn the focus regions. A very closely related approach to generate a saliency map was recently proposed by Anderson and Radic (2021), which in contrast to RISE and occlusion takes the physical meaning of the absolute value of each variable at each pixel into account during the perturbation of the input data.

One drawback of the 1D-CNN approach, as well as most other data-driven approaches, is the dependency on high data availability and quality. ~~In many areas~~ However, climate stations are often not available within the catchment ~~of a spring~~ itself, do not match the data availability of the discharge time series (period or temporal resolution), or are more distant and thus do not truly represent the ~~events in the catchment itself. For this, gridded~~ climatic conditions within the catchment. Gridded climate data can provide a solution ~~, with reasonable time periods and temporal resolutions being available from various products. Especially~~ to such data availability problems. Several openly available products exist (e.g. ERA5-Land (Muñoz Sabater, 2019), E-OBS (Cornes et al., 2018)), which provide climate data for several decades and with, in terms of karst spring modeling, appropriate temporal (hourly or daily) and spatial ($0.1° \times 0.1°$) resolution. However, especially for karst springs it is ~~difficult to simply extract corresponding~~ not straightforward to extract relevant time series from the gridded data, ~~since this requires knowledge of the spring catchment and usually the available grid cells do not exactly match the catchment either. Besides the modeling purpose~~ because the spatial extent of the grid cell containing the location of the spring, usually does not coincide well with the associated spring catchment position. Moreover, especially for karst springs, the catchment is often not well-known, and, for larger springs, can stretch over several grid cells. If the exact position of the catchment is unknown, using gridded data has the advantage that a broader region can be taken into account as input, to let the model learn the relevant grid cells automatically.

Besides such modeling aspects, the delineation of karst catchments is generally important to sustainably exploit but also protect karst water resources by establishing protection zones accordingly. Malard et al. (2015) explain that only few generalizable methods based on models in general for karst spring catchment delineation have been proposed. Instead, delineations usually rely on classical hydrogeological methods such as assessing geology, topography, hydrology, water balance, elaborate

95 tracer tests and geophysical investigations. These methods usually are complex and costly, thus for many karst springs, exact catchment delineations are not available at all or at least contain some uncertainties. Where no information about the catchment is available at all, an approximate localization is advantageous as a first step towards an exact delineation, since it facilitates the application of more elaborate methods like tracer test. There has already been an attempt by Longenecker et al. (2017) to semi-automatically derive approximate catchment boundaries by correlating karst spring discharge events with global precipitation

100 measurement (GPM) gridded data (NASA, 2016). The authors were able to achieve reasonable results with their method, but also noticed that they could not replace conventional methods.

Anderson and Radic (2021) ~~have~~ already applied gridded meteorological data to streamflow modeling in western Canada and used a ~~2D-CNN in combination with a long short-term memory (LSTM)~~ coupled 2D-CNN-LSTM model to directly ~~use~~ process spatially distributed input data. ~~LSTMs are recurrent neural networks, often used for time series modeling tasks.~~ They

105 showed that such models learn the relevant parts of the large scale gridded input data for each local or regional streamflow ~~by themselves~~automatically. We adapt and extent this approach to karst spring discharge modeling~~by establishing a similar model setup~~, however purely based on CNNs ~~, where a~~ by replacing the LSTM part with a 1D-CNN. Similar to the approach of Anderson and Radic (2021), in our proposed methodology the 2D-CNN ~~processes the spatially distributed input data~~and a subsequent part learns the spatial features of the input data, while the 1D-CNN ~~performs the forecasting of~~ part extracts

110 the temporal features, both necessary to simulate the spring discharge time series. With this combined 2D-1D-approach (for the sake of simplicity in the following only 2D-approach) we can now directly use gridded meteorological data to potentially overcome the common data availability problems ~~at climate stations, without the need for~~ when using climate station data for modeling. This approach further does not longer depend on a prior description of the catchment area, other than a very rough estimation of its approximate size to select the gridded data section large enough. Moreover, we investigate the potential of

115 this approach for identifying the approximate catchment location based on a modified spatial input sensitivity analysis from Anderson and Radic (2021). ~~Deriving~~ To derive recharge areas based on rainfall-discharge event correlation, as previously done by Longenecker et al. (2017), requires (i) heterogeneous rainfall at catchment scale, (ii) precipitation data with sufficient spatial resolution that capture this heterogeneity and (iii) a karst system without too much dampening of the precipitation signals. ~~This also applies to~~ These requirements hold for our proposed methodology ~~, although we expect ANNs being superior in~~

120 ~~representing non-linear~~ as well, but a potential advantage of ANNs is their nonlinearity which may better capture the nonlinear relationships between rainfall and discharge.

~~In total, we~~ We explore the applicability of our proposed deep learning approaches with spatially distributed input data in modeling karst spring discharge in three different study areas ~~. These study~~ in Austria (Aubach spring), France (Lez spring) and Slovenia (Unica springs). All three associated karst areas are well studied and for ~~two of them~~ Austria and France, several mod-

125 eling publications ~~, including also ANN approaches are available as benchmarks (Kong A Siou et al., 2011, 2012; Kong-A-Siou et al., 2013~~

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. We further are available as benchmarks. Discharge of Lez spring in France was extensively studied in the past, including several ANN studies. Please refer to Kong A Siou et al. (2011) for an overview about older modeling studies at Lez spring with approaches other than ANN. We omit three newer ANN studies because they either do not focus on modeling discharge (Kong-A-Siou et al., 2015) or train models not on the complete annual cycle (Sep.-Aug. in this region) but on flash-flood events (Darras et al., 2015, 2017). The other ANN studies all use classical multilayer perceptrons (MLP) or recurrent MLPs for discharge modeling and we introduce them shortly in the following. Kong A Siou et al. (2011, 2012) and Kong-A-Siou et al. (2013) use precipitation from three or six gauges, respectively, and all use a similar but slightly varying data basis of 12 to 13 full annual cycles between 1988 and 2006. Testing period is either the single cycle 2002/2003 (Kong A Siou et al., 2012; Kong-A-Siou et al., 2013) or two cycles roughly in the same period (2002-2004)(Kong A Siou et al., 2011). Kong-A-Siou et al. (2014) uses data from 1987 to 2007, however, this time additionally including evapotranspiration and pumping from the Lez aquifer. For Aubach spring in Austria no ANN studies exist, however, other modeling studies are available. Three studies (Chen and Goldscheider, 2014; Chen e... based on three successive and improved versions of a combined lumped parameter (SWMM) and distributed model, investigate and simulate three springs of this karst system simultaneously. They all achieve high performance in terms of NSE (>0.8), but none of them covered a complete annual cycle as contiguous test period. Additionally, they differ considerably in terms of their individual data basis for modeling (number and position of climate stations used as input data), as well as their testing periods. The shortest test set only had 40 days (in autumn), the longest (Chen et al., 2017b) used one year of data for model calibration and performed a split-sample test on the same data set. This makes a comparison of modeling results among these studies difficult. For the third spring (Slovenia), several earlier modeling studies are available (e.g. Kaufmann et al., 2016; Mayaud et al., 2019; Kau... , even including ANNs (Sezen et al., 2019), but none of these directly modeled Unica springs discharge, but rather focused on other aspects like cave hydraulics or polje modeling. Besides existing studies we compare the results of the 2D-model with own 1D-CNN models using conventional climate station input data to assess the usefulness and possible advantages of the direct use of spatially distributed input data. As spatially distributed inputs we use either hourly ERA5-Land reanalysis data (Muñoz Sabater, 2019) or daily E-OBS data (Cornes et al., 2018), depending on the temporal resolution of spring discharge data. We selected these datasets among all openly accessible datasets (e.g. via Copernicus Climate Data Store), because of their available variable set and their spatial and temporal resolution. We introduce them in more detail in the following data section. Finally, we explore the potential of the 2D-approach for karst spring catchment localization by investigating the spatial input sensitivity of the trained CNN models.

2 Data and Study Areas

2.1 Overview

In this study, we investigate three different karst springs: Aubach spring in the Hochifen-Gottesacker area in Austria (Fig. 1a), springs of Unica river in Slovenia (Fig. 1b) and Lez spring in southern France (Fig. 1c). All springs show different characteristics regarding relevant system properties (e.g. catchment size, complexity of the hydrological system), environmental conditions (e.g. dominant climate, anthropogenic forcing) and data availability (see also Table A1). Furthermore, all All areas

are well studied ~~,~~ and existing data was easily accessible~~and except Unica~~. Further, several previous modeling approaches are available for comparison~~.~~, except for the Slovenian spring.
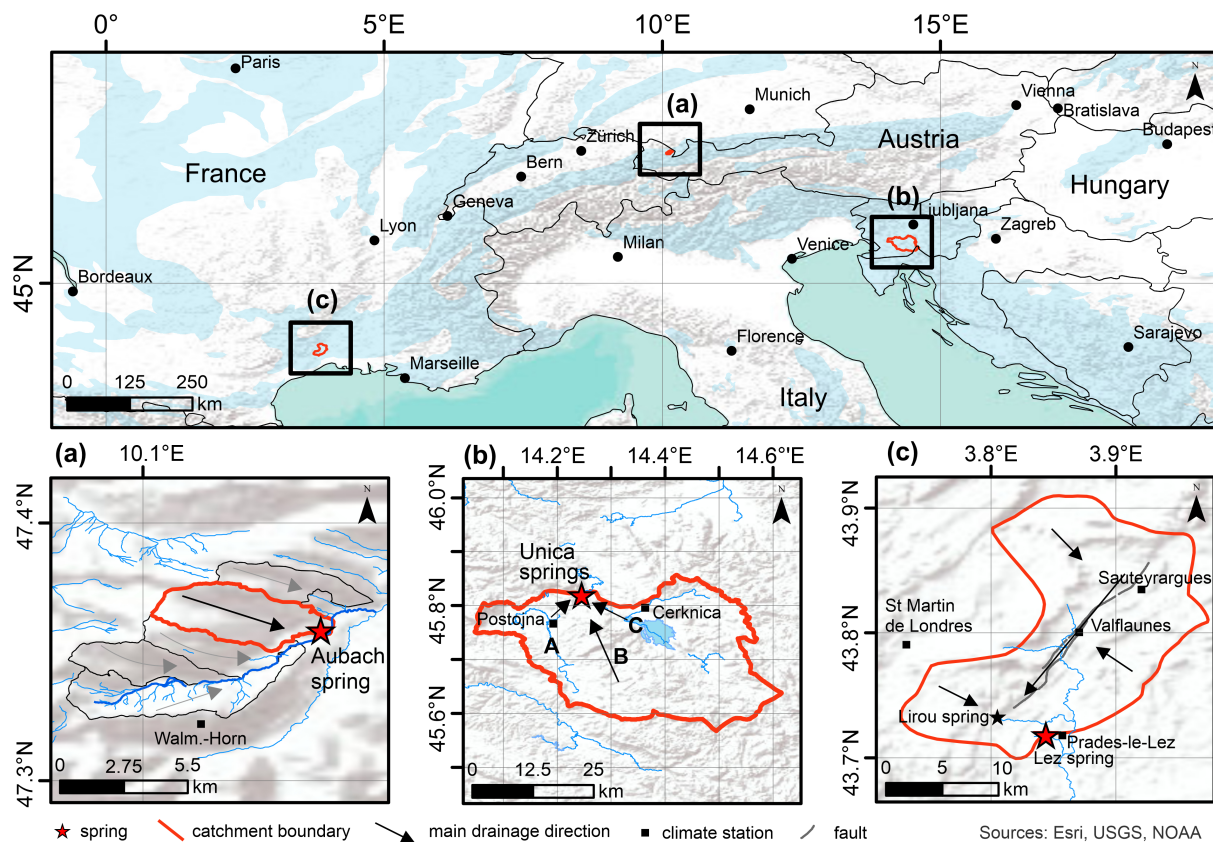
Figure 1. Overview of all three study areas, the simulated springs (red star) and their catchments (red lines). Black squares indicate the locations of climate stations used for 1D-modeling (~~not all~~ some are outside the shown ~~in these~~ maps), blue shadings in the upper map show karst areas based on WOKAM (Chen et al., 2017a) (a) Hochifen-Gottesacker karst area and Aubach spring, black lines depict minor contributing sub-catchments; (b) Unica river springs and Javorniki karst plateau (B); (c) Lez spring catchment, Lirou overflow spring (black star) and major fault Corconne-Les Matelles (grey line);

2.2 Aubach Spring, Austria

Aubach spring is a major karst spring in the Hochifen-Gottesacker karst area in the northern Alps at the border between Germany and Austria. Southern border of the area is the Schwarzwasser valley, which geologically forms the contact zone between the Helvetic Säntis nappe in the north and sedimentary rocks of the Flysch zone in the south (Goldscheider, 2005). In the northern part the dominant karst formation is the Schrattenkalk formation, a cretaceous limestone with a thickness of about 100 m. This Schrattenkalk is structured in folds, which hydrogeologically form parallel sub-catchments (Fig. 1a) that contribute to different proportions to the several springs in the valley (Goldscheider, 2005; Chen and Goldscheider, 2014). In this study

we focus on one large, non-permanent spring called Aubach spring (1080 m asl, discharge up to 10 m^3/s). The Hochifen-Gottesacker area is largely influenced by seasonal snow accumulation and melting in the elevated regions (>1,600 m asl),
which is also clearly reflected in the discharge of Aubach spring by increased baseflow and ~~daily~~ diurnal snowmelt-induced variations, especially in the months of April to June. Earlier studies by Goldscheider (2005) and Chen and Goldscheider (2014) have identified one major catchment area of Aubach spring with approximately 9 km^2 (Fig. 1a), still, to smaller ~~parts~~ proportions upstream catchments can also contribute to Aubach spring discharge depending on the flow conditions. This applies also to the non-karstified Flysch area directly in the South (southernmost sub-catchment in Fig. 1a), where precipitation events are only relevant during low flow conditions. Then, the surface runoff from this area sinks into an upstream estavelle and contributes via an underground connection to the discharge of Aubach spring. During high flow conditions, the estavelle itself acts as an overflow spring and no contribution from surface runoff at Aubach spring occurs. Generally, the climate in the area can be described as cooltemperate and humid and the mean annual precipitation at the closest used climate station in this study (Walmendinger Horn) is about 2000 mm (2003-2019).

For this study ~~Aubach spring is selected~~ we select Aubach spring because of the good data availability ~~. We~~ and use 8 years of hourly discharge data provided by the office of the federal state of Vorarlberg, division of water management~~, and we further use~~. Further precipitation and temperature data from three surrounding climate stations are available: Oberstdorf, Walmendinger Horn (shown in Fig. 1a) and Diedamskopf. Additionally, due to the high importance of snow in the area, we run a snowmelt routine as preprocessing of the meteorological input data as described in Chen et al. (2018). This routine is a slightly modified version (after Hock, 1999) of the HBV hydrological model snow routine ~~(e.g. Bergström, 1975, 1995; Kollat et al., 2012; Seibert, 2000)~~ (e.g. Bergström, 1975, 1995; Kollat et al., 2012; Seibert, 2000), which redistributes the precipitation time series in accordance with probable snow accumulation and snowmelt.

2.3 Unica Springs, Slovenia

The Unica springs (450 m asl) are located on the southern edge of a karst polje in SW Slovenia and are important from a biodiversity and water supply perspective. There are two permanent and several temporary springs that feed the Unica river. The joint discharge during 1989-2018 ranged from 1 to 90 m^3/s, while the mean discharge was 21 m^3/s (ARSO, 2020a). The springs are fed by three clearly distinguishable sub-catchments covering an area of about 820 km^2. The main recharge area is the highly karstified Javorniki plateau (up to 1,800~~m~~ m asl; marked B on Fig. 1b), whose predominant lithology is Cretaceous rocks~~,~~; mainly limestones, changing in places to dolomites and breccias. To a lesser extent, Jurassic and Palaeogene carbonate rocks are also present. The thickness of the unsaturated zone is estimated to be up to several hundred meters (Petrič et al., 2018, and references therein). To the east, a strike-slip fault zone controls the hydrology of the area~~is controlled by a strike-slip fault zone~~, along which a chain of karst poljes developed (between 500 and 700 m asl; marked C on Fig. 1b). Upper Triassic dolomites predominate, changing to Jurassic limestones and dolomites in the south and west, forming aquifers with fracture porosity, which in places have very low to moderate permeability, and in some parts a superficial river network forms. As the karst poljes follow each other in a downward series, they are connected in a common hydrological system with transitions between surface and groundwater flows, and frequent flooding (Mayaud et al., 2019). In the ~~west~~West, the Pivka River Basin

(between 500 and 700 m ~~asl~~; marked A on Fig.1b) consists of poorly permeable Eocene ~~flysch in the north~~Flysch in the North, which conditions a surface river network. The southern part consists of Cretaceous and Jurassic carbonate rocks forming a shallow karst aquifer. Surface flow ~~occur~~ occurs during high water levels, receiving additional water from intermittent springs on the western foothills of the Javorniki plateau. The water flow of the sinking rivers in the subsurface from the regions A and C ~~parts is clearly~~ is of the channel flow type. ~~The springs were selected~~ We select the springs for this study because they drain a complex binary karst system of the so-called ~~Classical Karst~~classical karst, they are well studied with ~~a large amount~~ long records of hydro-meteorological data and their hydrology is influenced by substantial snow accumulation and melting. The catchment belongs to the moderate continental climate and is mostly covered with forests. For this study we use daily discharge data from the Unica-Hasberg gauging station (in the following called Unica) (ARSO, 2020a) and daily meteorological data from Postojna and Cerknica ~~meteorological~~ climate stations ranging from 1981 to 2018 (ARSO, 2020b). ~~The meteorological~~ These climate stations (squares in Fig. 1b) are located on the western (Postojna) and eastern (Cerknica) part of the catchment, representing different climate regimes and are separated by the karst massif in between. For Postojna station the following ~~parameters~~ variables are available: precipitation (P), temperature (T), potential evapotranspiration (PET), relative humidity (rH), snow (S) and new snow (nS). For Cerknica station only P, S and nS ~~are available~~exist. Average annual precipitation during 1989-2018 is about 1500 mm and on average ~~, there are~~ 33 days of snow cover ~~per year~~ occur in Postojna (530 m ~~)~~asl) per year, while even longer snow cover is expected on the plateau.

2.4 Lez Spring, France

Our third study area is located 15 km north of Montpellier in southern France, within a large and complex karst system delimited by rivers and marly terrains. Eastern and western borders are the Vidourle and Hérault river valleys, northern and southern borders are piezometric limits. At larger scale, northern and southern boundaries are structural boundaries due to Cévennes and Montpellier faults, respectively. The dominant karst formations are Argovian to Kimmeridgian, and Berriasian massive limestones with 650 m to 1000 m thickness. Infiltration occurs mostly diffuse but also localized through fractures and sinkholes along the basin and through the major geologic fault of Corconne-Les Matelles in the northern part of the basin (indicated by a grey line in Fig. 1c).

The hydrogeological basin associated to the Lez spring has ~~been estimated to be~~ a size of about 240 km^2 (Fig. 1c), which is estimated on the basis of the hydrodynamic response to high discharge continuous pumping into the saturated zone of the aquifer (Thiéry and Bérard, 1983). However, the effective recharge catchment of the Lez spring, which corresponds to the extent of Jurassic limestone outcrops, has been estimated to be about 130 km^2 (Fleury et al., 2009; Jourde et al., 2014). The Lez karst aquifer is under anthropogenic pressure (i.e. aquifer exploitation for water supply) with pumping performed directly within the karst conduit. The discharge is measured at the spring pool and is regularly null during low water periods, when the pumping rate exceeds the natural spring discharge. Ecological water discharge towards the Lez river (160 L/s then 230 L/s after 2018) is ensured during such periods by a partial deviation of the pumped water to the river. Lirou spring (Fig. 1c) is the main of several overflow springs that activate during high flow periods (Jourde et al., 2014).

The Lez catchment is exposed to a Mediterranean climate, ~~which is~~ characterized by hot and dry summers, mild winters and wet autumns. Analyses by MeteoFrance show that on average 40% of the annual precipitation occurs between September and November with a high variability across years (Bicalho et al., 2012). The average annual rainfall rate for the 2008-2018 period is 904 mm.

For this study, ~~the modeling is based on~~ we use nearly 10 years of daily discharge data provided by SNO KARST (Jourde et al., 2018; SNO KARST, 2021). The temperature data is from the Prades-le-Lez climate station; we use, however, an interpolated precipitation data series that is derived from a weighted average of four rainfall stations (Fig. 1c) (similar to Fleury et al., 2009; Mazzilli et al., 2011), three of them being located on the Lez catchment (Prades-le-Lez, Valflaunès, Sauteyrargues). The fourth station (Saint-Martin-de-Londres) is located few kilometers west of the catchment. Interpolation is in principle possible in this area due to the existing topography; at the same time, interpolation based on Thiessen-polygons (compare Appendix B) also allows compensation for data gaps at single stations. We decided to apply this preprocessing, because all but Saint-Martin-de-Londres climate station show such gaps from time to time, which explains the benefit from including within-catchment precipitation. ~~Including pumping data is not favorable~~ We do not use pumping data as input in this study, because these were only available for a shorter period of time and such data would also not be available for a real forecast in the future (in ~~contrary~~ contrast to weather and climate data).

~~For Lez spring, results from several existing modeling approaches, including several ANN studies, are available. Please refer to Kong A Siou et al. (2011) for an overview about older modeling studies at Lez spring with different approaches. Here, we focus on the most recent studies for comparison, all of which were conducted with ANNs (Kong A Siou et al., 2011, 2012; Kong-A-Siou et . These studies are based on modeling Lez spring using Multi-Layer-Perceptrons (MLP) or recurrent MLPs. They use a wide variation of daily data from different time periods and also have different study goals. Darras et al. (2015, 2017) focus only on single events to evaluate flash flood forecasting, while Kong-A-Siou et al. (2013, 2014) and Kong-A-Siou et al. (2015) can be best compared to the work presented here.~~

2.5 Spatial Climate Data

Besides climate station data, we explored raster data from the E-OBS (Cornes et al., 2018), the ERA5-Land (Muñoz Sabater, 2019) and from the RADOLAN ~~(?)~~ (DWD Climate Data Center (CDC), 2020) as spatially distributed model inputs. E-OBS provides daily gridded meteorological data for Europe from 1950 to present, derived from in-situ observations, ERA5-Land provides hourly reanalysis data from 1981 to present. Both are available with a spatial resolution of $0.1°° \times 0.1°°$ (approx. 8 km $\times$ 11 km for all study areas). Depending on the dataset, different sets of ~~parameters~~ variables are available. In case of E-OBS we initially provide our models with precipitation (P), mean, minimum and maximum temperature (T, Tmin, Tmax), relative humidity (rH) and surface shortwave downwelling radiation (Rad). For ERA5-Land, where a substantially larger set of ~~parameters~~ variables is available, the following were used as initial inputs: total precipitation (P), 2m temperature (T), total evaporation (E), snowmelt (SMLT), snowfall (SF) and volumetric soil water of all four available layers (SWVL1: 0 - 7 cm, SWVL2: 7 - 28 cm, SWVL3: 28 - 100 cm, SWVL4: 100 - 289 cm). Relevant input ~~parameters~~ variables from both datasets are later selected through Bayesian optimization (see section 3.3). The spatial extent of the input data is chosen very generously

for each spring, so that between 6 and 8 additional cells are available as input data around the respective catchments. This prevents a predefinition of the area that needs to be identified as relevant as well as reduces the influence of possible border effects due to the CNN approach using 3x3 filters (compare methodology section). The resolution of ERA5-Land and E-OBS data corresponds to the grid cell size shown in the catchment plots in Figures 1a-c, although each showing a slightly different absolute position of their grid center points. ~~We already see that the relation of grid resolution to catchment size varies strongly, with Aubach catchment being the smallest and Unica catchment being the largest.~~ Depending on the temporal resolution of the available spring discharge measurements, we choose the spatial input data in accordance, thus E-OBS for Unica and Lez spring, ERA5-Land for Aubach spring.

Compared to the catchment size of Aubach spring (about $9\,\mathrm{km}^2$), the spatial resolution (approx. 8 km ~~x~~ $\times$ 11 km) of the gridded input data is extremely coarse. We therefore additionally explore a combination of ERA5-Land input ~~parameters~~ variables (except P) with radar based precipitation data (RADOLAN) that offers a spatial resolution of 1 km ~~x~~ $\times$ 1 km ~~(?). For each of the RADOLAN grid cells, the according parameter value of the ERA5-Land data is chosen, where the RADOLAN grid cell center lies in. This corresponds to the simplest form of downscaling. For this analysis,~~ (DWD Climate Data Center (CDC), 2020). The higher resolved precipitation data from RADOLAN is thus augmented with climate variable values from ERA5-Land (for T, rH, etc.), which were downscaled and re-gridded to match the $1 \times 1\,\mathrm{km}^2$ RADOLAN grid. Compared to the ERA5-Land section around Aubach spring, for this additional analysis we reduce the spatial extent of the 2D-input data to save calculation time, but ~~increase the~~ still considerably increase the total number of cells ~~compared to the ERA5 section around Aubach spring~~ due to the higher resolution of the RADOLAN grid.

3 Methodology

3.1 Modeling Approach

In this study, we simulate karst spring discharge with deep learning models using meteorological input data. As proof of feasibility, we use meteorological data from surrounding climate stations as inputs to 1D-CNN models. However, ~~these stations often show limited data availability in terms of the number of parameters (mostly limited~~ data from such stations are often limited to precipitation and temperature, rarely more~~), the record length,~~, as well as ~~the sampling interval~~ often exhibit data gaps, and limited record length or coarse sampling intervals. Also, the ~~spatial coverage and proximity is often unsatisfactory~~ proximity to the catchment is often not sufficient, which especially in mountainous regions can introduce a distinct error ~~of parameters with high~~ in representing the true conditions within the catchment. This applies especially to variables with higher spatial variability such as precipitation.

Gridded meteorological data can ~~offer~~ be a solution to these issues, as they usually provide good temporal coverage and ~~resolution, a reasonable~~ sampling intervals, a good spatial resolution as well as a large-scale availability (e.g. continental (E-OBS) or even global ~~) availability~~ (ERA5-Land), see Bandhauer et al. (2021) for a comparison of both products). Further, especially reanalysis data include a larger ~~parameter set. However, when~~ variable set. When the catchment of the spring is unknown, it remains unclear which cells ~~to retrieve time series from when using 1D-time series as inputs~~ of the gridded data

should be selected to best represent the climate conditions in the catchment, because the actual location of the spring is only a very rough indicator for the location of the catchment. Based on our revised version of the approach of Anderson and Radic (2021), we demonstrate a solution by processing 2D-inputs and letting the model decide ~~by itself~~automatically, which parts of the input data are relevant to model the spring discharge.

3.2 Convolutional Neural Networks (CNN)

Convolutional ~~Neural Networks~~ neural networks (LeCun et al., 2015) are widely applied in several domains such as object recognition (e.g. Cai et al., 2016), image classification (e.g. Li et al., 2014), and signal ~~processing~~or natural language processing (e.g. Yin et al., 2017; Kiranyaz et al., 2019). The structure of most CNN models is based on the repetition of blocks that are made up of several layers, typically at least one convolutional layer followed by a pooling layer. The former matches the dimension of the input data (e.g. 2D for image alike data, 1D for sequences such as time series) and uses filters with a fixed size (receptive field) to produce feature maps of the input. The latter performs down-sampling of the produced feature maps and ~~hence increases the density of information~~summarizes the features detected in the input. This decreases the total number of parameters of the model and makes it approximately invariant to small translations of the input (Goodfellow et al., 2016). A large variety of model structures based on such blocks, in combination with additional layers in between to prevent exploding gradients (e.g. batch normalization layers (Ioffe and Szegedy, 2015)) or model overfitting (e.g. dropout layers (Srivastava et al., 2014)) are possible; however CNNs usually end with one or several fully connected dense layers to produce a meaningful output.

From ~~our experience in preliminary work and~~ earlier studies (Wunsch et al., 2021; Jeannin et al., 2021) we know that 1D-CNNs are fast, reliable and excellently suited for modeling hydrogeological time series, such as groundwater levels or spring discharge. We have shown that they are faster compared to LSTMs, which are often the method of choice for time series modeling, and even outperform them or at least show similar performance (Wunsch et al., 2021). This is in agreement with the findings of (Van et al., 2020) in the domain of rainfall-runoff modeling. ~~We therefore perform~~ In Wunsch et al. (2021) we further show that for the closely related application of groundwater level forecasting, CNNs are less sensitive to the random initialization procedure and thus provide more stable results. Based on these findings we choose CNNs for predicting karst spring discharge ~~modeling in~~ in this study and establish two different setups. One setup uses 1D-meteorological input data from surrounding climate stations ~~, the other one uses gridded climate data as input and thus combines the~~ and applies a 1D-CNN ~~model with a time distributed~~ for forecasting. The second approach consistently uses a 1D-CNN to learn temporal features for discharge prediction, but combined with a time-distributed 2D-CNN ~~model. The 2D-CNN model processes the spatially distributed input data, while the~~ to learn spatial features directly from gridded climate input data. Compared to the approach in Anderson and Radic (2021) we replace the LSTM by a 1D-CNN ~~is used for time series forecasting in both setups~~to make both setups methodologically consistent. Using CNNs in both setups further helps to assess the influence of using spatially distributed input data in terms of model accuracy, as we do not have to speculate if higher or lower performance might be due to the LSTM model rather than the input data. ~~Using a 1D-CNN subsequent to the 2D model instead of a LSTM, as in Anderson and Radic (2021) for example, makes both setups methodologically consistent and improves the comparability~~
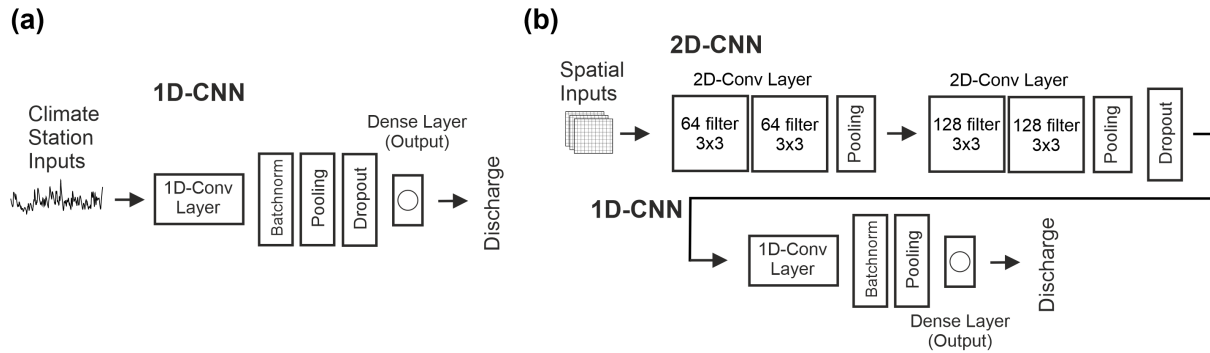
Figure 2. Model structures applied for modeling karst spring discharge based on climate station data (a) and gridded meteorological input data (b). Flatten layers are not displayed.

~~among them.~~ The general model structure of both setups is shown in Figure 2. They basically use the same 1D-model except the position of the dropout layer. We use Bayesian hyperparameter optimization to select the 1D-filter number, batch-size and input sequence length of each model in both setups.

To reduce the dependency on the random initialization of the models, we use an ensemble with 10 members, each based on a different pseudo-random seed. Further, we implement Monte-Carlo dropout to estimate the model uncertainty from a distribution of 100 results for each of the ten realizations of each model in this study. We derived the 95% confidence interval from these 100 realizations by using 1.96 times the standard deviation of the resulting distribution for each time step. Each uncertainty was propagated while calculating the overall ensemble mean value for final evaluation in the test set. This uncertainty is shown as confidence interval for each of our simulation results in the following. We want to point out, that this uncertainty does not include other sources (such as input data uncertainty) but the random number dependency. All our models are implemented in Python 3.8 (van Rossum, 1995) and we use the following libraries and frameworks: Numpy (van der Walt et al., 2011), Pandas (McKinney, 2010; Reback et al., 2020), Scikit-Learn (Pedregosa et al., 2011), Unumpy (Lebigot, 2010), Matplotlib (Hunter, 2007), BayesOpt (Nogueira, 2014), TensorFlow and its Keras API (Abadi et al., 2015; Chollet, 2015).

3.3 Model Calibration and Evaluation

We split the time series data for each site into four parts according to Table 1. While the first part is used for training, the second part (validation) is simultaneously used to prevent the model from overfitting via early stopping. The model's hyperparameters are optimized according to its performance on the optimization set, while the last set is used as completely independent test set for final evaluation of the model performance without data leakage from training or optimization. Training epoch number and early stopping patience are varied manually for each model at each test site. Hyperparameters for the 1D-CNNs of both setups are optimized on the respective optimization set as stated above, maximizing the sum of Nash-Sutcliffe efficiency and R^2 (calculated as explained below). The number of optimization steps is also varied manually for each model and is always a trade-off between accuracy and computational costs. In case of many available input ~~parameters~~ variables we treat input ~~parameter~~

Table 1. Data splitting schemes for all study areas (number of values in parentheses).

	Time Interval	Training	Validation	Optimization	Testing
Aubach spring	Hourly	2012-2017	2018	2019	2020
		(44,807)	(8,760)	(8,760)	(7,320)
Unica spring	Daily	1981-2012	2013+2014	2015+2016	2017+2018
		(11,687)	(730)	(731)	(730)
Lez spring	Daily	2008-2016	2017	2018	2019
		(2,629)	(366)	(365)	(701)

variable selection equally as a global optimization problem and use Bayesian optimization to simultaneously select a proper set of input ~~parameters~~ variables and hyperparameters. Thus, input optimization is used for each 2D-model, as ERA5-Land and

360   E-OBS offer several different ~~meteorological parameters~~climate variables, as well as to the 1D-model of Unica springs, where the climate station records provide additional climate variables such as snow cover. For Lez spring and Aubach spring, only a smaller input ~~parameter~~ variable set is available ~~and~~ (mainly precipitation and temperature) and hence fully used. For all models we ~~offer~~ use an additional input (Tsin), which is a ~~sinus~~ sine curve fitted to the temperature data. This ~~parameter~~ variable can provide the model with noise-free information on seasonality and on the current position in the annual cycle (Kong-A-Siou

365   et al., 2014). Precipitation is the only ~~parameter~~ variable that is not optimized but fixed as input, because it has undoubtedly ~~the most important~~ major influence on the discharge of a karst spring. The optimized hyperparameters, information on some fixed hyperparameters, and a summary of the number of parameters in each model, is given in Appendix Table D1.

We calculate several metrics to evaluate the performance of our models: Nash-Sutcliffe Efficiency (NSE) (Nash and Sutcliffe, 1970), squared Pearson r (R^2), root mean squared error (RMSE), Bias (Bias) as well as Kling-Gupta-Efficiency (KGE) (Gupta

370   et al., 2009). For squared Pearson r we use the notation of the coefficient of determination (R^2), because we compare the linear fit between simulated and observed discharge, thus of a simple linear model, which makes them equal in this case.

3.4   Spatial Input Sensitivity and Catchment Localization

Anderson and Radic (2021) show in their study that ~~when using 2D-input data for CNNs for streamflow modeling, there is physical meaning in the way that spatial fractions of the input data are learned to be more important than others~~combined

375   2D-CNN-LSTM models can learn to focus on specific areas of the spatially distributed input data and that these make physically sense. We modify this approach and transfer it to karst spring modeling, where we demonstrate that this approach ~~to qualitatively localize karst catchment locations~~is suited to approximate the location of karst catchments.

We use the Gaussian spatial perturbation approach from Anderson and Radic (2021), which is similar to other input sensitivity algorithms such as occlusion (Zeiler and Fergus, 2014) or RISE (Petsiuk et al., 2018), but in contrary to these methods

380   takes into account the physical meaning of the absolute ~~parameter value for each~~ value of each variable at each pixel during the perturbation. We modify this approach so that only a single ~~channel (input parameter,~~ input channel (e.g. precipitation) is

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perturbed at a time for the sensitivity analysis. For details of this approach we refer to the original study. In short it works by perturbing spatial fractions of the input data by adding or subtracting a 2D-Gaussian curve from the input data at a certain location. ~~The perturbed data is~~ Both the perturbed and unperturbed data are passed through the trained model to determine the resulting ~~error from the specific perturbation~~ simulation error between them. In this way, after many ~~repetitions~~ iterations, heat maps are created that show how sensitive the trained model is to perturbations of certain areas of the input data. ~~In the case of karst spring modeling we perturb only single channels, instead of all channels at once as in the original approach, for the following reasons. We use some very different input parameters and ideally want to separate the individual influence of each of these channels. Also these parameters show a very different~~

The considered input variables in our study show different properties in terms of spatial heterogeneity and variability~~(i. e. spatial autocorrelation), which means that the model can learn the importance for example of temperature from a large area~~. Temperature for example usually exhibits a distinct spatial autocorrelation, ~~as long as it favors a lower simulation error, while for precipitation ideally a smaller area corresponding to the catchment should have a higher influence on the spring discharge and therefore has to be learned more accurately. The intended use for catchment localization, which especially in Karst areas is driven by precipitation predominantly, makes it necessary~~ meaning that temperature information from outside the catchment area may be used to infer temperature within the catchment area. In contrast, precipitation is less spatially autocorrelated, meaning that precipitation information from outside the catchment area is less related to precipitation from inside the catchment area. Therefore, we hypothesize that the within-catchment precipitation fields will be most important for the model's prediction, and we will test this hypothesis by visually inspecting the sensitivity maps produced by the modified approach of Anderson and Radic (2021). Compared to the original approach by Anderson and Radic (2021), we therefore perturb only single channels at a time, instead of all channels at once, to separate the influence of each channel on the model output.

4 Results and Discussion

4.1 Aubach Spring

Figure 3a shows the simulation results of the 1D-CNN model for the test period 2020, using only available climate station input data. Error measures indicate a high accuracy of the model simulation~~,~~: NSE and R^2 values both are 0.74, KGE is 0.79. We observe that peaks in winter and spring are underestimated~~but the~~. The snowmelt period, clearly visible by increased baseflow and ~~daily~~ diurnal variations from April to June, is nicely fitted, as well as the following summer peaks. A short series of discharge peaks in the end of September/beginning of October is not captured. We assume that these were caused by small-scale precipitation events that are not represented in the data of the climate stations used as inputs. Interestingly, ~~daily~~ diurnal variations, which might be learned during the snowmelt period, are also visible in periods not influenced by snow (e.g. in August). From ~~experience (Chen et al., 2017b)~~ Chen et al. (2017b) we know the high relevance of snow in this area and by coupling the CNN model with a snow routine data preprocessing, we are able to further improve the model performance (Fig. 3b). We now can achieve a fit with 0.77 for both NSE and R^2, KGE increases to 0.84. Our model is able to ~~nicely~~ better fit the

second largest peak of the whole dataset, which occurs in February, though, the peak is slightly overestimated, whereas other peaks still tend to be underestimated. The snowmelt period remains well simulated, but shows increasing deviations close the end of the period. The earlier noticed ~~daily~~ diurnal variations in summer and autumn, now ~~no longer appear~~are diminished, which is ~~most certainly~~ presumably an effect of the snowmelt preprocessing.

Please note that the 95% model uncertainty from random number dependency, estimated from 10 differently initialized models with a Monte-Carlo dropout distribution from 100 runs each (i.e. 1000 simulations in total), is very low for both modeling results (a+b) compared to the overall variability of the discharge. ~~In general, we~~ We assume the spatially limited input data to be the major source of ~~uncertainty, as~~ error in the complete modeling procedure, because all climate stations ~~have a certain distance to~~ are located outside of the catchment area ~~; however, as explained in the methods section, such uncertainty is not included in the confidence interval shown in the plots~~and thus introduce distinct uncertainty about the true conditions within the catchment. Other modeling approaches ~~(Chen and Goldscheider, 2014; Chen et al., 2017b, 2018) based on three successive and improved versions of a~~ (Chen and Goldscheider, 2014; Chen et al., 2017b, 2018) based on combined lumped parameter (SWMM) and distributed ~~model~~models, achieve similar or higher NSE values for the simulation of Aubach spring discharge (0.92, 0.83, 0.80 respectively)~~but in contrary to our approach simulate three springs simultaneously. However, these results are~~. As mentioned, the results are, however, hardly comparable with each other and neither with this study. Reasons are (i) different ~~data basis regarding the~~ input data (number and position of climate stations~~used as input data~~), (ii) different simulation periods~~as well as~~, and (iii) very different test set lengths. ~~The shortest test set only had 40 days (in autumn), the longest (Chen et al., 2017b) used one year of data for model calibration and performed a split-sample test on the same data set. Despite our model shows a slightly lower NSE value compared to these three models, it is in the same range and we assume it to perform at least equally as~~ One reason for the slightly lower performance of our model could be that none of the previous studies covered a complete annual cycle as contiguous test period, including high peaks in late winter and strong snowmelt influence in spring and early summer.

Figure 3c shows the results of the 2D-modeling setup using (only) ERA5-land input data. Based on ~~Bayesian optimization , besides the fixed and not optimized input P, the following input parameters are selected:~~ the described optimization procedure, the model uses the following inputs: P, T, E, SMLT, SWVL2 and SWVL4 (for a comparison of selected ~~parameters~~input variables with other study areas see also Table A1). The performance of the 2D-model is similar to that of the 1D-models, showing a NSE (0.76) and RMSE in-between both, a larger R^2 (0.8) but a lower KGE (0.71). This performance is still high considering that the major catchment is extremely small (about $9\,km^2$) compared to one ERA5-Land grid cell, and that a large grid section of 14 ~~x~~$\times$ 14 ERA5-Land cells (1.4° ~~x~~$\times$ 1.4°) was used as input. We see that the major peak in February is slightly underestimated, as well as the beginning of the snowmelt period in April; however, the end of this period in May/June has improved now compared to (b). Both 1D-models are superior in estimating the peaks especially during summer, except the already mentioned peaks in September/October, which have improved using the 2D-input data. This supports the assumption that the climate stations do not represent these precipitation events, but the 2D-data does due to its spatial nature.

To account for the small area of the catchment of Aubach spring, Figure 3d shows the results of the 2D-input data, using the spatially higher resolved RADOLAN precipitation data in combination with downscaled ERA5-Land data~~for all other~~
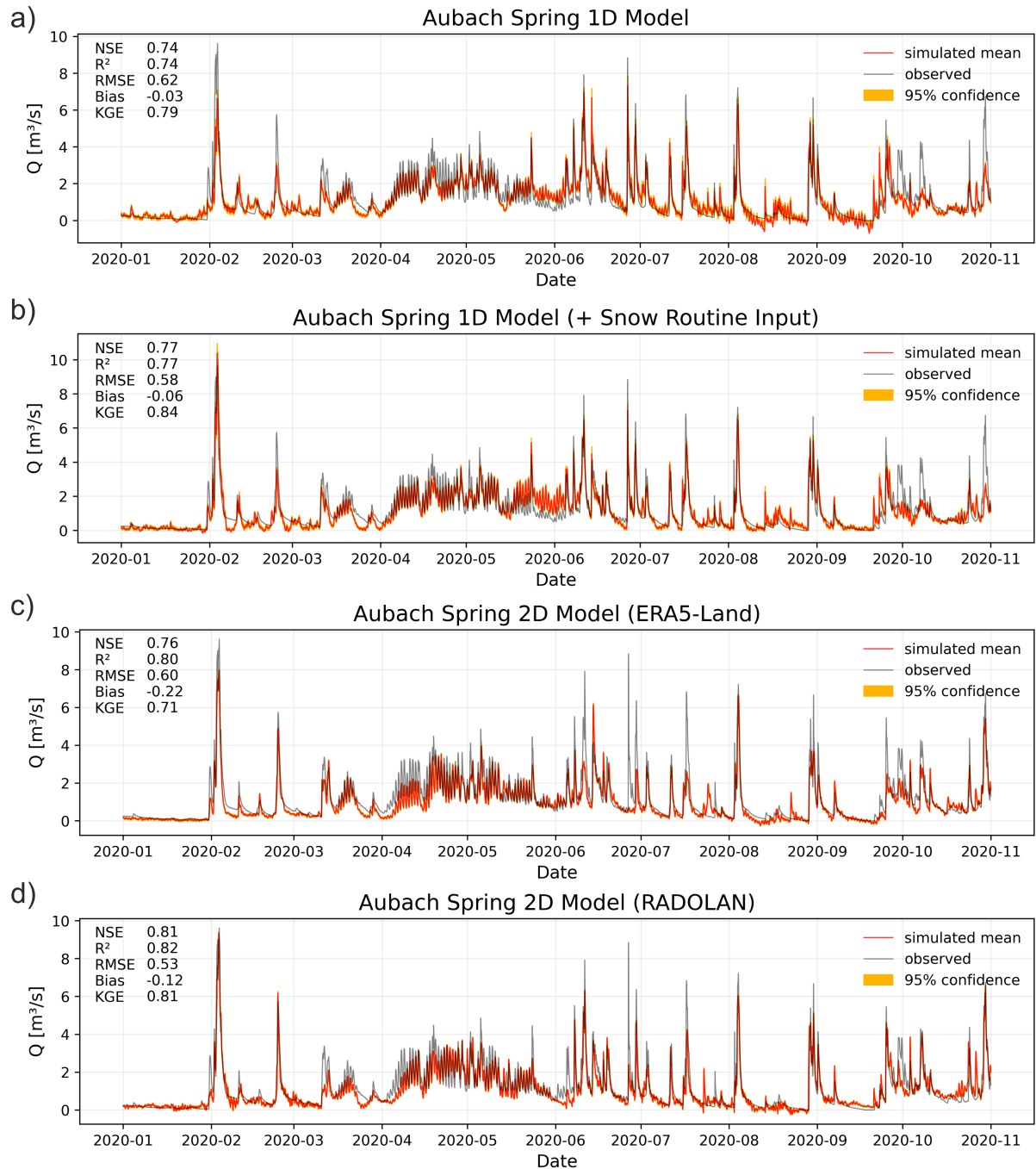
Figure 3. Simulation results for the year 2020 at Aubach spring: (a) 1D-model based on climate station inputs, (b) 1D-model with additional snow routine preprocessing, (c) 2D-model based on ERA5-Land gridded data and (d) 2D-model with combination of ERA5-Land data and RADOLAN precipitation input.

450 ~~parameters~~. We have reduced the spatial extent of the 2D-input, but ~~use an even higher~~ still have a reasonable buffer around the catchments and, compared to the former 2D-model, increase the grid cell number considerably ($22 ~~\times~~ \times 22$ or 22^2 km²)~~, with a reasonable buffer around the catchments. Additionally to P, the~~. The optimized model uses ~~inputs from all available parameters except E and SWVL3, thus~~ P, T, Tsin, SMLT, SF, SWVL1/2/~~4.~~4 as inputs, thus omits E and SWVL3. This model shows the best performance of all four models by reaching a NSE of 0.81, R^2 of 0.82 and KGE of 0.81. Similar to the model in (c), the

455 beginning of the snowmelt period in April remains slightly underestimated and compared to the ~~1D models~~ 1D-models, the peaks in summer are less well fitted. Nevertheless, we generally see an accurate fit, especially the largest peak in February is well ~~represented~~reproduced. Compared to the 1D-approach, the main source of uncertainty for both 2D-models should be the uncertainty of ~~parameter values resulting from the ERA5-land grid cell sizes, which is too large compared~~ ERA5-Land variables. Their values originate from large grid cells in comparison to the catchment size~~. Improved~~, thus it is not clear

460 how well they represent the true conditions on catchment scale. A more elaborated downscaling of ERA5 data or other high resolved climate data for a combination with RADOLAN precipitation data might be a promising approach for simulating small catchments like this one. Model uncertainty derived from random number effects and Monte Carlo dropout is (equally to the 1D-models) satisfyingly small. In total~~we see~~, we think that both the 1D and the ~~2D approach~~ 2D-approach for this catchment bear substantial ~~uncertainties~~ shortcomings in terms of ~~input data~~how well the input data represents the true conditions in

465 the catchment, even though the simulation results are generally very accurate. On the one hand the climate stations represent the true observed climate, on the other hand this is true only for a very specific point, which is in this case ~~even~~outside the catchment, and embedded into a highly variable topography. The ~~2D data, however, shows too large grid cell sizes for~~ 2D-data have a too coarse spatial resolution compared to the size of the Aubach spring catchment and ~~is itself~~ are themselves modeled (in case of ERA5-Land). We therefore do not think that one approach is superior ~~in terms of uncertainty~~ for this study area,

470 but we can show that even in this case with relatively ~~course~~ coarsely gridded input data compared to the catchment size, the 2D-approach offers a decent alternative in case of missing climate station data.

4.2 Unica Springs

Figure 4 summarizes the 1D- and 2D-model performance on the years 2017 and 2018 for Unica springs in Slovenia. The simulation of this quite large catchment area (820 km²) is based on the data of only two climate stations (Postojna and Cerknica).

475 All available input ~~parameters~~ variables from both stations except relative humidity from Postojna station and new snow from Cerknica station were used as inputs as selected by the Bayesian optimization model. The 1D-model shows ~~solid~~ good performance overall (NSE: 0.73, R^2: 0.79, KGE: 0.63), including ~~reaction~~ a response for all major discharge events. However, ~~recessions~~ recession slopes especially in 2017 are ~~estimated substantially too conservative~~underestimated substantially and the plateau shapes of the large peaks (e.g. January 2018) are not well captured, but rather simulated as multiple peaks. In general,

480 many of the high flow events at this gauge have a quite long duration of days to even weeks resulting in such plateau-like shapes. This is due to the regular flooding of the polje. After the drainage areas of the polje are completely flooded, there is a progressive back-flooding and a steady rise in the water level, which makes it impossible to accurately monitor the ~~inflow conditions~~ flow conditions under these conditions. Therefore, ~~simulating multiple peaks~~during the plateau-like peaks, when

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we cannot observe the true flow; the peaks simulated by the ANN might be conceptually ~~even more truethan the plateau-like shape, however not easy~~ true, which is however not possible to evaluate. The peak in April 2018 is quite clearly underestimated, whereas the following low flow period (summer 2018) is slightly overestimated. ~~One possible reason could be~~ Such overestimation might be due to small scale meteorological events that are detected by the climate stations, but do not well represent the conditions in the whole catchment area. It is also important to notice that during 2014 and 2018 substantial environmental changes ~~that~~ occurred in the catchment ~~during 2014-18~~ (Kovačič et al., 2020). During this period a considerable amount of vegetation was destroyed by a series of large-scale forest disturbances. We expect the evapotranspiration changed due to changes in canopy interception, water use, and soil moisture. As a result, spring behavior has likely changed, because vegetation cover is an important element of the water balance and recharge events may have resulted in higher infiltration rates and more intense spring response, as well as more pronounced droughts. ~~Because the period prior to 2014 was~~ The effect of this environmental change on the model performance is hard to evaluate, because it is not part of the training data ~~(1981-2012), the change in spring behavior could not be predicted, resulting in an observed modeling incompatibility~~. However, the model was optimized and validated (early stopping) on a part of the period with environmental changes, which means that the model may infer some information on the changes from these periods (2014-2016). It is not expedient to exclude this change from model building, since this would require to shorten the time series to the period after 2018, thus loosing almost the complete data basis. Due to highly complex hydraulic behavior in this study area, which is for example related to ~~large~~ already mentioned polje floodings and to a strongly variable water level in the system that varies also the catchment area, extracting the highly non-linear precipitation-discharge is especially challenging. We generally observe less dynamics in terms of the number of flood pulse events compared to Aubach spring. In terms of intensity of hydrologic variability, discharge rates can vary by ~~many~~ about two orders of magnitude. This is primarily due to the large size of the catchment area, the very high degree of karstification of the carbonate rocks, and the fact that the main spring may acts as an overflow spring.

By using the 2D-input data from 18 ~~x~~ × 21 E-OBS grid cells we were able to improve the model performance substantially (Fig. 4b), ~~showing~~ reaching now a NSE of 0.83, a R^2 of 0.84 and a KGE of 0.80. ~~Selected input parameters~~ Model input variables are: P ~~(fixed)~~, Tmax, rH and Rad. We generally observe a similar shape of the simulation as for the 1D-model but with overall reduced errors. Still, the plateau ~~shape~~ shapes of some peaks ~~is~~ are not well captured, but the same conceptual understanding as for the 1D-model seems to be learned. ~~Recessions are generally too conservative,~~ which means the model mainly simulates peaks instead of plateau-shaped high-flow events. The slope of the recessions are still generally underestimated, especially the simulation of low flow periods and minor discharge events improve clearly though. ~~These~~ The improved results are plausible, ~~as minor discharge peaks are presumably due to small precipitation events , which may not be reflected in the selected climate station data , but visible in the~~ because we can expect precipitation events to be represented more accurately in the gridded data ~~derived from a larger set of observational points~~ that in the point data of only two climate stations, especially considering the size of the catchment. As for Aubach spring, both models show a comparably low model uncertainty based on random number variation and Monte-Carlo dropout, the model uncertainty of the 2D-simulation is even a bit lower than for the 1D-model. Again, we assume the spatially limited climate station data to be the main source of data uncertainty in the 1D-model, because meteorological stations are located on the western and eastern side of the karst ~~massive. The~~
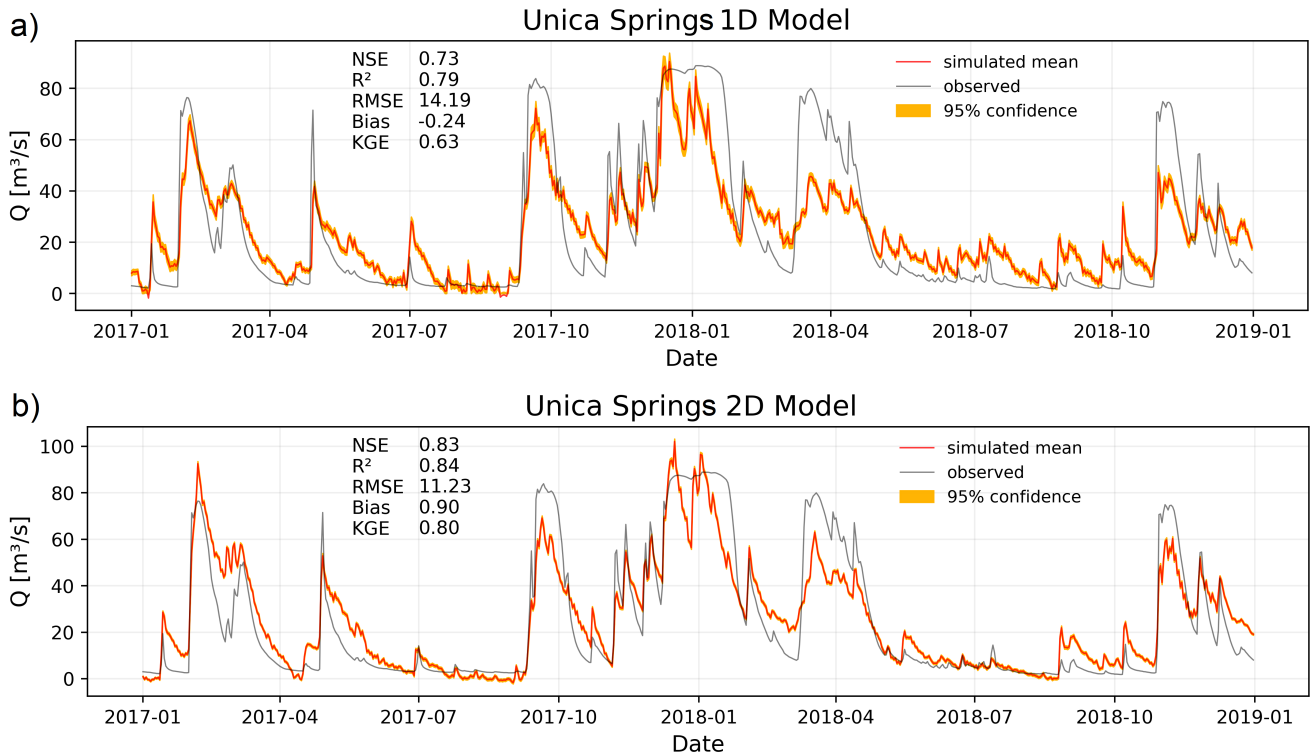
Figure 4. Simulation results for 2017-2018 at Unica springs in Slovenia using climate station input data (a) and E-OBS gridded data (b).

~~karst massive~~ massif. The massif itself represents the orographic barrier with different temperature and precipitation regimes
520   that are certainly not captured by the considered meteorological stations. ~~For 2D-data, the general grid uncertainty may be comparably low due to the large size of the catchment. Several earlier modeling studies were conducted in the area of the Unica catchment (e.g. Kaufmann et al., 2016; Mayaud et al., 2019; Kaufman et al., 2020; Kovačič et al., 2020) even including ANNs (Sezen et al., 2019), but none of these directly modeled Unica springs discharge, but rather focused on other aspects like cave hydraulics or polje modeling.~~ Concerning the 2D data, the grid resolution is sufficiently high to adequately represent the
525   climatic conditions in this large size catchment.

4.3   Lez Spring

Lez spring represents a third class of study area, as the catchment size (around $240\,km^2$) is somewhere in between the two others, the climate is Mediterranean and the spring runs dry for a considerable amount of time during the annual cycle due to a constant exploitation of the karst aquifer through pumping. Figure 5 shows both the results for the 1D- (a) and the 2D-model
530   (b). Despite comparably short training (daily data, starting in 2008) we observe a very high fit of the 1D-model above 0.86

for NSE, R^2 and KGE. As well the timing of the peaks, the absolute height of the peaks, as the dry periods are simulated accurately, except some deviations in early 2019.

For the 2D-model we use input data from 19 ~~x~~× 18 E-OBS grid cells and the Bayesian model selects only rH and Rad as inputs besides the fixed input P. Considering the high relevance of potential evapotranspiration ~~in Mediterranean areas, this should be easily learnable from relative humidity and radiation data~~(PET) in the Mediterranean, it is a bit surprising that temperature, as a major driver of PET, is not selected (neither T, Tmin nor Tmax). However, relative humidity is also important to calculate PET (King et al., 2015) (e.g. low rH favors high evaporation) and the information on seasonality well encoded in a temperature time series, is presumably deducible from the radiation data (higher in summer than in winter) . The performance of the model is ~~basically~~ very good, but clearly lower compared to the 1D-model, showing NSE, R^2 and KGE between 0.75 and 0.78. Generally, ~~2018 is better simulated than~~ the simulation is better in 2018 than in 2019, which is~~however also slightly visible for~~, however, also a tendency of the 1D-model. ~~Some~~ The model simulated some non-existent peaks ~~are simulated by the model~~ in the dry sections, after all one of them (in Oct. 2018) ~~is also simulated by~~ clearly occurs also in the 1D-model's simulation. Presumably, ~~these differences in performance can be explained by~~ the input data is accountable for the general performance differences between both modeling approaches. The climate stations, from which the interpolated precipitation time series is derived, are mainly located inside the catchment and additionally represent a good spatial coverage. Compared to both other study areas~~the 1D input uncertainty is definitely the lowest for Lez spring catchment. Though, it seems~~, the 1D-input data here best represents the climatic conditions within the catchment. Based on the lower performance of the 2D-model, we conclude that it seems to be harder to extract the relevant ~~data~~ relationships between climate forcing and spring discharge from the gridded data~~, which~~. This may be related to ~~uncertainties from the~~ a less favorable ratio of grid cell size ~~in relation~~ to the catchment size~~(e.g. which may be more important than for Unica but way less than for Aubach). Nevertheless, the~~, than for the Unica catchment for example. The model uncertainty based on initializations and derived from Monte-Carlo dropout again is small for both model setups, especially during dry periods.

~~Several other modeling approaches exist for comparison at Lez spring, of which we refer to three especially suited studies in the following. Kong-A-Siou et al. (2013) used a 1-year test set in 2002-2003 and obtained the highest NSE of all studies (0.96~~The results of our models (1D-NSE: 0.87, 2D-NSE:0.75) can compete with the results from several earlier studies (NSE: 0.76-0.88 (Kong A Siou et al., 2011), NSE: 0.76-079 (Kong-A-Siou et al., 2014)), however~~the focus of the study was knowledge extraction from the ANN. Kong-A-Siou et al. (2014) simulated the period from October 2003 to August 2004~~, we do not beat the maximum performance reported by Kong A Siou et al. (2012) (NSE: ~~0.85) and Kong-A-Siou et al. (2015) investigated different years between 1997 and 2004 with strongly varying NSEvalues ranging from 0.1 to 0.85. Compared to our study, usually a larger database was used for training in these studies, which in itself is a plausible reason for the good performance. Most studies put substantial effort into the consideration of evapotranspiration or potential evaporation, further sometimes pumping data from the accompanying wells was also used as an input, which we, however, did not include~~ 0.69-0.95) and Kong-A-Siou et al. (2013) (NSE: 0.96). Generally, all studies, including ours, achieve high performance and it is hard to conclude reasons for the superiority of one or other study, as several factors differ among them, such as model types, training and testing periods, or set of input variables. For our study, we chose not to include pumping data (as used

20
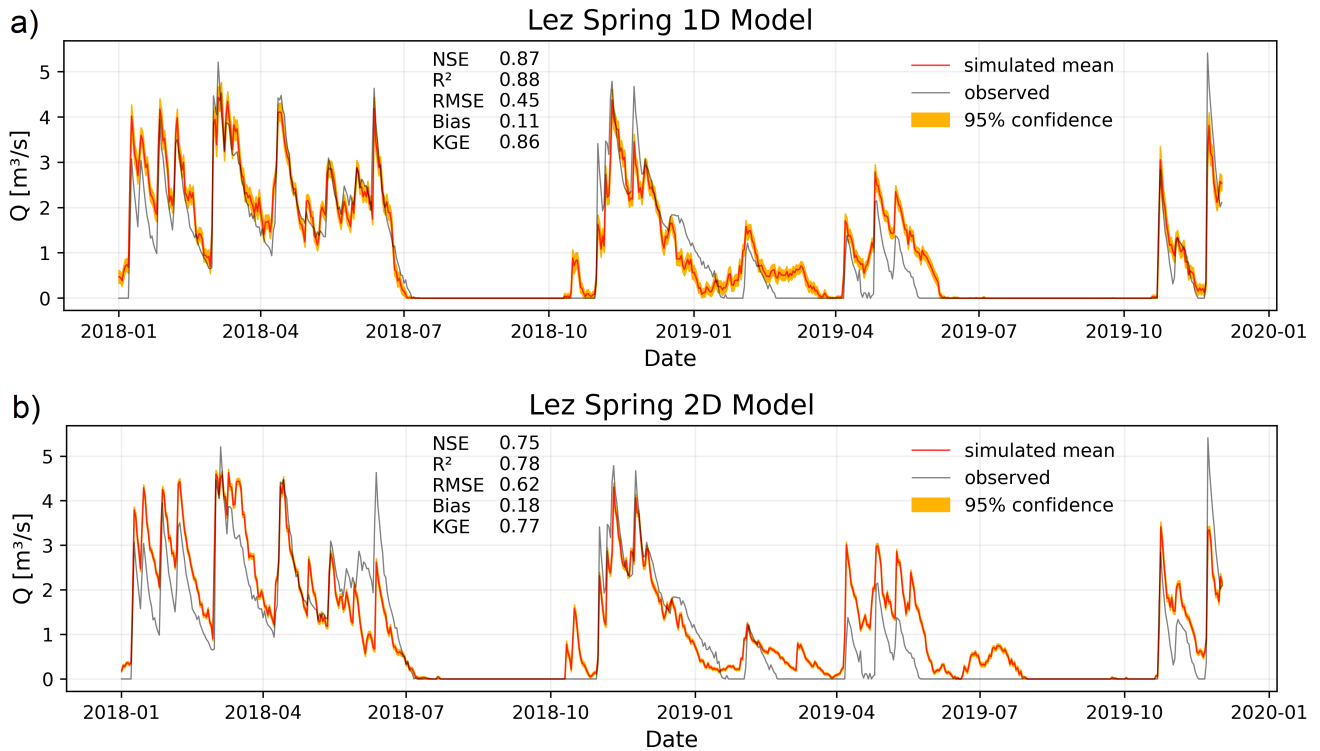
Figure 5. Simulation results for 2018-2019 at Lez spring in France using climate station input data (a) and E-OBS gridded data (b).

in (Kong-A-Siou et al., 2014)) due to the data availability reasons elaborated in section 2.4, as well as to be consistent in the ~~2D modeling~~ 2D-modeling approach, which would need an update of the model structure due the 1D-time series character of the pumping data. ~~Despite limited comparability, we nevertheless can conclude that our 1D-CNN models can compete with the performance of these earlier ANN approaches even though we do not beat the best NSE value from these studies due to~~ 570 ~~the fact that we use less and differing input data for our 1D-model.~~ The 2D-approach still shows very ~~solid performance in~~ ~~comparison, but cannot fully compete with the 1D-model and earlier ANN approaches~~good performance in general, however, in comparison among all mentioned NSE values its performance is rather low. Nevertheless, we ~~also show that it would offer~~ ~~a solid substitute of the 1D-model~~ conclude if no climate ~~stations were available~~ station data would be available to apply a 1D-model, the 2D-approach still offers a reasonable substitute.

575   4.4   Spatial Input Sensitivity Results

The most important results of the spatial input sensitivity analysis from all catchments are shown in Figure 6. In case of Aubach spring modeled with ERA5-Land data (Fig. 6a), we can see that the catchment is ~~hardly the size of~~ smaller than one grid cell. Hence, despite the quite ~~solid~~ good discharge modeling, we see no clear spatial meaning of the precipitation channel

heatmap. We also find a border effect with an almost uniform decrease in sensitivity toward the edges, which is an important reason to choose the spatial extent of the data large enough. This effect could be related to the size of the filter in the convolutional layer (3×3), as it sometimes only occurs in the one or two outermost pixels (e.g. Fig. 6c). In combination with zero-padding, which we apply to improve the informative value of the edges and to maintain the data size throughout the convolutions, this may result in such error halo, as also illustrated by Innamorati et al. (2020). Yet its origin remains unclear and not all heatmaps show this pattern (Fig. 6d), which questions the hypothesis of being a purely technical issue. For Aubach spring, precipitation shows only the fourth highest sensitivity (S) in terms of absolute values, while the second most sensitive variable is snowmelt (SMLT), which shows also the best spatial agreement with the catchment area. This is plausible insofar as the discharge for a large part of the time is dominated by snowmelt and to a lesser extent directly by precipitation. We conclude that even though the modeling results are satisfying, not much meaning can be extracted from the spatial sensitivity analysis for such a small catchment, given the existing spatial resolution of the gridded data. Please find heatmaps of all other variables in Appendix Figure C1. The combined approach of RADOLAN and ERA5-Land data (Fig. 6b) shows the heatmap in more detail in relation to the size of the catchment. We show only the precipitation heatmap, because it is the only variable with a native resolution of 1 km $\times$ 1 km and we do not consider the spatial patterns of the remaining ERA5-Land-based variables to be meaningful to interpret. We observe that the most sensitive cells are identified close to the spring and at the border between the main catchment and the southern adjacent subcatchment. Due to the small scale of the spatial extent shown in Fig. 6b in relation to the spatial extent of precipitation events, the model is not able to sharply distinguish between precipitation inside and outside the catchment. This is presumably also related to the data, as precipitation is not directly measured, but estimated from radar signals and subsequently adjusted according to measured values from nearby climate stations. It remains unclear if precipitation is spatially resolved with sufficient accuracy in such alpine valleys on km-scale. No plausible reasoning exists for the two separate sensitive areas in the SW and NE corners, however, they are less sensitive then the center cells of the map.

Heatmaps of all four selected E-OBS variables at Unica catchment are shown in Figure 6c. In accordance with our expectation for karst areas, we see the highest sensitivity for precipitation, which visually also identifies the catchment area very well. Especially Tmax and rH show high sensitivities on larger areas, however they are usually highly spatially autocorrelated and do not show a strong spatial heterogeneity like precipitation, which makes it plausible that the model learns from larger areas and does not concentrate strongly on the catchment itself. The model further identifies an area in the north as most sensitive for radiation.

Heatmaps of the 2D-Lez spring model are shown in Figure 6d. In this area the model very strongly ignores large parts of the input data (dark blue, no visible border effects) and comparably sharply identifies the relevant area for the spring. This might be related to the higher spatial heterogeneity of precipitation in Mediterranean climate (Fresnay et al., 2012), which in this specific region has a special

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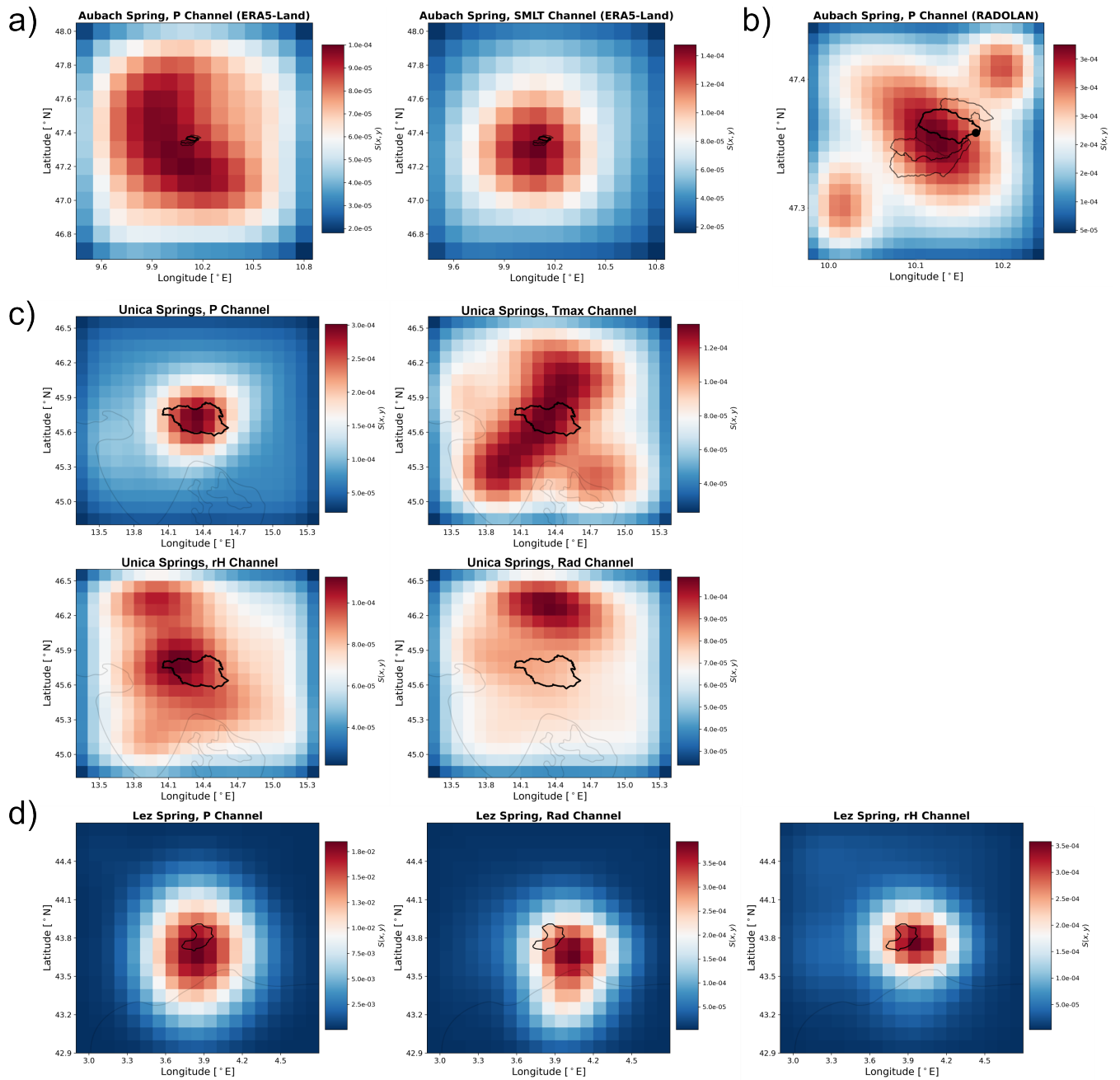
Figure 6. Heatmaps of spatial input sensitivity for Aubach spring based on ERA5-Land gridded data (a), for Aubach spring based on RADOLAN precipitation data (b), Unica springs (c) and Lez spring (d) both based on E-OBS gridded data. In case of (c) and (d), light-grey lines indicate the coastlines for orientation.

importance (severe flash floods known as Cévenol episodes (Kong A Siou et al., 2011)). Generally, we observe a slight south and east shift of the highest sensitivity compared to the catchment position. This might be related to the performance of the 2D-approach, which could not compete with the 1D-models. Maybe the model did not exactly learn the most relevant ~~input fraction~~spatial features. The most sensitive ~~parameter~~ variable is precipitation, while the rH channel shows the best spatial fit. We furthermore see that the size of the catchment is about the minimum size to produce meaningful heatmaps based on this given grid resolution, which corresponds also to our interpretation of the 2D-model performance shortcomings in comparison with the 1D-approach.

Given the spatial resolution of the used input data, the obtained heatmaps, and the simulation results of all three catchments, the ~~size of the~~ Unica springs catchment seems to be most appropriate to further investigate the usefulness for catchment localization. ~~We conducted~~ It has the highest ratio of catchment size to data resolution and exhibits both generally high performance of the ANN models, and especially a considerably improved performance when using spatially distributed inputs compared to climate station input data. Thus, we used the Unica springs to conduct additional experiments to investigate the sensitivity of our approach to the absolute catchment location within the ~~selected spatial dataframe~~considered area of the input data. Figure 7 shows the results of these experiments, where we shifted the ~~2D input~~ 2D-input data boundaries in such a way that the catchment is located in one of the four corners or edges, leading to eight additional modeling results, named by the position of the catchment in the ~~data frame~~ considered area of the input data. (e.g. *upleft*: catchment in the upper left corner). First of all, we find that all models ~~are similarly able to extract the relevant input data and thus~~ successfully model the spring discharge curve ~~.~~ and similarly learn the relevant grid cells of the considered input area, i.e. they are able to learn the approximate position of the catchment. The NSE values vary moderately between 0.80 and 0.85 among all models. ~~Moreover, the~~ The heatmaps of the precipitation input channel visually well identify the location of the catchment for each of the different ~~data frames used~~considered areas of the input data. We find that regardless of the catchment's position within the ~~data frame~~considered areas of the input data, the resulting high-sensitive area in the P channel ~~is very similar~~well indicates the true catchment position. For the heatmaps of the other input channels, we see that usually larger areas are identified as relevant and more variations between the models occur. Two things are particularly noticeable here. First, the identified sensitive input areas are generally slightly smaller for the *up** models, which is possibly related to the fact that the ~~data frame~~ considered area of the input data is shifted towards the Mediterranean Sea, where no input data are available in the E-OBS dataset (compare the grey coastline). These areas contain zeros or mean values and show no temporal variation that could be used to model the spring discharge. Second, the noticeably best performing model (*downleft*, NSE of 0.85) is the model with the least fraction of no-data cells (due to the Sea)~~in the data frame~~. Intuitively, we would not have expected the best performance here, but rather with the *upright* model, since there it is almost predetermined where the model has to learn. So the model seems to be able to use the larger amount of "useful data", even outside the catchment, to improve the overall performance. To possibly delineate a catchment from these results, a strategy has to be developed regarding the sensitivity contrast between the catchment and its surroundings. From our results we conclude that focusing on the precipitation channel is the most promising approach for potential catchment delineation. This makes, however, only sense if (i) precipitation is sufficiently heterogeneous at the scale of investigation, ~~and~~ (ii) if conceptually spring discharge is mainly driven by precipitation (not snowmelt for example) and

(iii) the gridded climate data is provided in a relatively high spatial resolution compared to the catchment size. Please find the precipitation channel heatmaps for Aubach spring and Lez spring in Appendix Figures C2 and C3.

In summary, we observe that the approach in its current form can produce meaningful heatmaps for at least roughly locating karst spring catchments. At least for the precipitation channel, we showed that the location of the catchment is successfully learned, regardless of the position within the ~~selected spatial dataframe~~considered area of the input data, if the ratio of catchment size to grid cell size is favorable (as for Unica springs). We notice that it generally works better the larger the catchment area, especially in relation to the grid cell size, but the absolute size of the catchment itself appears to be also important. For small catchments it seems harder to extract precise catchment locations, even if spatially finer-resolved data are available. This might be related to the fact that at small scales, even precipitation has a distinct spatial correlation, which can lead to higher sensitivity also in areas outside the catchment. However, one should keep in mind that these conclusions are only tendencies as we only investigated a small number of catchments. To develop a catchment delineation strategy, future investigations should analyze more catchments with adequate ratio of size to grid cell resolution, such as Unica catchment. Moreover, it can be expected that more and better gridded meteorological data products will be available in the future, which might lead to better results with the proposed methodology also for catchments with varying sizes.

5 Conclusions

From the obtained insights we can conclude that karst spring discharge can be predicted accurately with the presented 1D and ~~2D approaches. Their accuracy rivals~~ 2D-approaches. Their performance competes with that of existing models in the three study areas~~, with the difference that~~. One main advantage compared to conventional modeling approaches in karst is that in order to obtain precise discharge simulations, far less prior knowledge of the system under consideration is required~~than, e. g., for lumped parameter models. This can substantially~~. Thus, using ANNs can generally reduce the amount of ~~work required, provided that a mere simulation of the spring discharge is the objective~~preliminary work that would be required to gain such sufficient system knowledge. We can further show that gridded climate data can provide an excellent substitute for non-existent or patchy climate station data. This does not require knowledge of the exact catchment area, which is a critical component especially for karst springs. Rather, ~~2D-CNNs~~ coupled 2D-1D-CNNs can be used to generate a first approximation of the catchment location. However, ~~this approach is subject to some inaccuracies and~~ as it was shown, this approach still needs further development ~~in combination with~~ to more accurately localize the catchment, for example by modifying the input sensitivity approach and by defining a routine to infer the catchment location from the sensitivity data, other than visual inspection. An important factor to achieve more accurate catchment localization is 2D-meteorological input data ~~in~~ with a finer spatial resolution in relation to the catchment size, because we found the approach to work best for the largest catchment. Additionally, a sufficient heterogeneity of precipitation in comparison to the catchment size is necessary~~. Then, we assume it can be used to delineate catchments quite accurately, which can then be evaluated~~, which, however, cannot be controlled, but possibly limits the application in some karst areas. Given these developments and conditions, the approach's capabilities to delineate karst catchments should be further investigated, ideally including an evaluation against tracer tests and hydrogeological studies. In
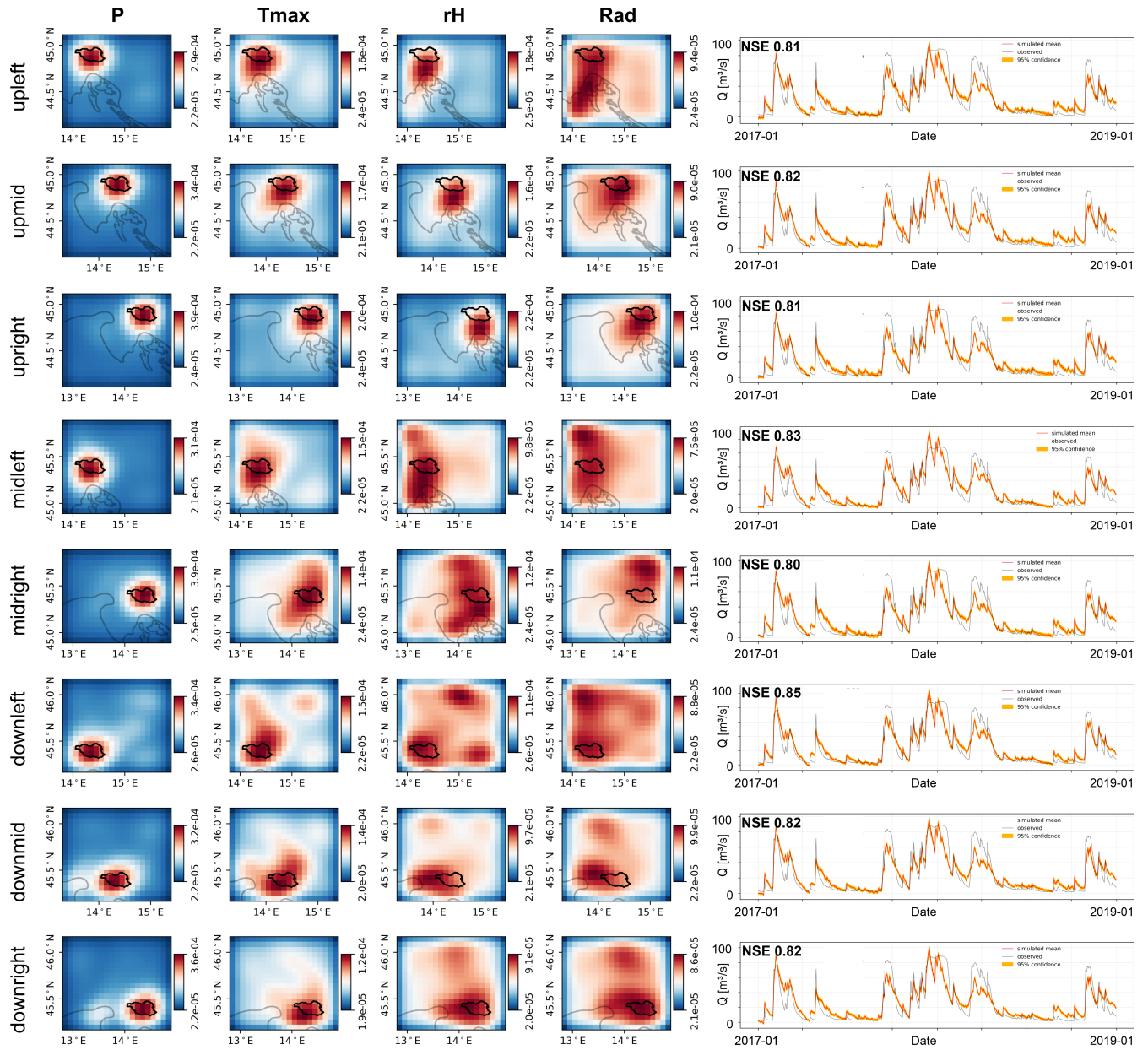
Figure 7. Heatmaps of spatial input sensitivity for Unica springs catchment based on E-OBS gridded data. The considered area of the gridded input data section is shifted to demonstrate the spatial learning capabilities of the models.

terms of accuracy, we do not find that one of the tested model setups (1D and 2D) is fundamentally superior. ~~Nevertheless, we would conclude that~~ A key benefit of the 2D-approach~~is superior to the 1D-approach with respect to the effort of data collection as well as data and parameter availability. Though, a substantially increased computational effort is necessary for the~~

685 ~~training as well as for the optimization of~~ , which uses spatially discretized input data, is the ~~models~~spatially and temporally complete nature of the data and the number of variables available for study. Furthermore, for many areas the openly available 2D-climate data are easier accessible than climate station data, which still have to be collected from various different authorities, if accessible or existing at all. A weak spot of the 2D-approach is a substantially higher computational effort due to the large number of model parameters and the larger amount of data that has to be processed during training and optimization. In

690 summary, gridded meteorological data is ~~excellently~~ useful to overcome missing climate station data and to get a quite good idea of the spatial extent of larger catchments~~in relation to the grid cell size~~, given sufficiently small grid cell sizes.

Code and data availability. We provide complete model codes on Github (AndreasWunsch/CNN_KarstSpringModeling) (Wunsch, 2021). Due to redistribution restrictions from several parties we cannot provide a dataset. Nevertheless, the data is available from the respective local authorities listed in the main text and in the following. 2D-datasets (E-OBS, ERA5-Land) are fully accesible online via Copernicus

695 (cds.climate.copernicus.eu). Aubach spring discharge and climate data from surrounding climate stations in Austria are availble on request from the office of the federal state of Vorarlberg, division of water management, Oberstdorf station data (German Meteorological Service) is available online (opendata.dwd.de). Data from Slovenia can be retrieved from ARSO (Slovenian Environment Agency)(ARSO, 2020a, b). Lez spring discharge was provided by SNO KARST (2021), climate data is available on request from MeteoFrance.

Appendix A: Study Area Comparison Table

Table A1. Summary and comparison of different aspects of all three study areas.

	Aubach Spring	Unica Springs	Lez Springs
Country	Austria	Slovenia	France
Climate	cooltemperate and humid	moderate continental	mediterranean
Catchment Area [km^2]	9	820	240
mean Precipitation [mm/year]	2000	1500	904
Station, Period	(Walm.-Horn, 2003-2019)	(1989-2018)	(2008-2018)
spatially distributed input datasets	ERA5-Land, RADOLAN	E-OBS	E-OBS
Offered ~~Parameters~~ variables	P, T, Tsin, E, SMLT, SF, SWVL1-4	P, T, Tmin, Tmax, Tsin, rH, Rad	P, T, Tmin, Tmax, Tsin, rH, Rad
Selected ~~Parameters~~ variables	ERA5-Model: P, T, E, SMLT, SWVL2, 4 RADOLAN-Model: P, T, Tsin, SMLT, SF, SWVL1, 2, 4	P, Tmax, rH, Rad	P, rH, Rad
Omitted ~~Parameters~~ variables	ERA5-Model: Tsin, SF, SWVL1, 3 RADOLAN-Model: E, SWVL3	T, Tmin, Tsin	T, Tmin, Tmax, Tsin

Appendix B: Lez Catchment Precipitation Interpolation

The Thiessen's polygon interpolation method consists of calculating a weighted average of the precipitation data by allocating a contribution percentage to each meteorological station, based on its influence area on the catchment. These influence areas are calculated through geometric operations. First, we draw straight-line segments between each adjacent station, then we add the perpendicular bisectors of each segment, which will define the edges of the polygons. Each meteorological station thus corresponds to a particular polygon, for which the precipitation over the surface is assumed to be the same as the measured precipitation at the station.
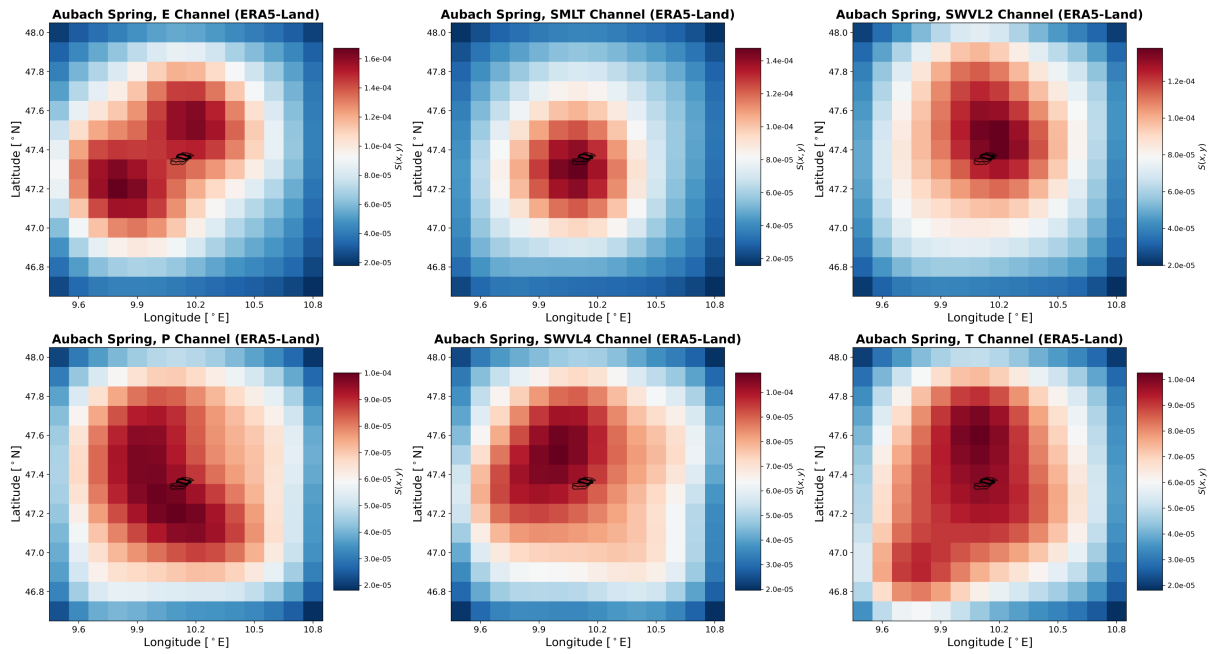
The weighted average of the precipitation P_{wa} at each time step is calculated as follows:
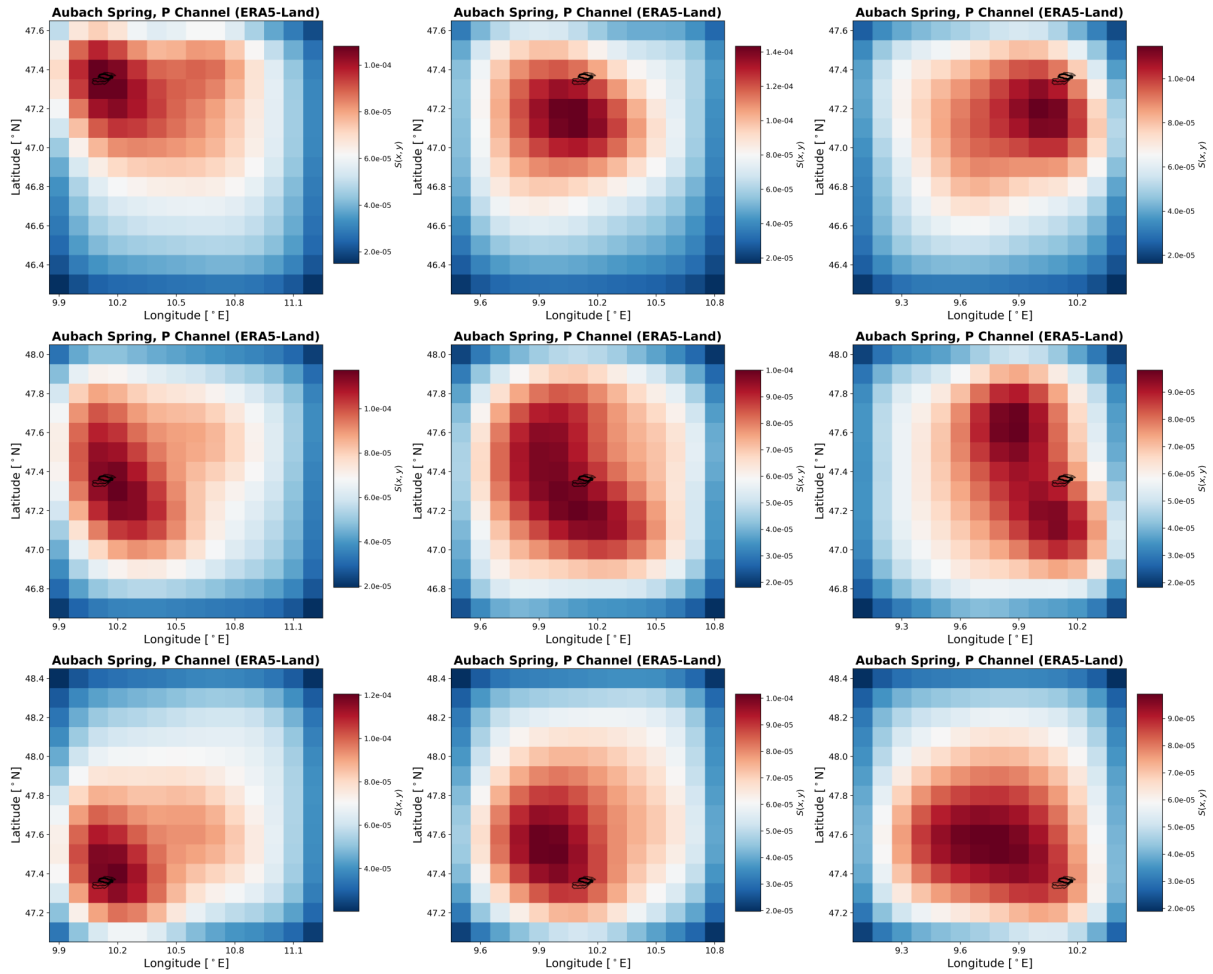
$$P_{wa} = \frac{\sum_{i=1}^{n} A_i P_i}{A} \tag{B1}$$

With n the number of meteorological stations, A_i the area (over the catchment) of the polygon corresponding to the ith station, P_i the precipitation measured at the ith station and A the area of the catchment.
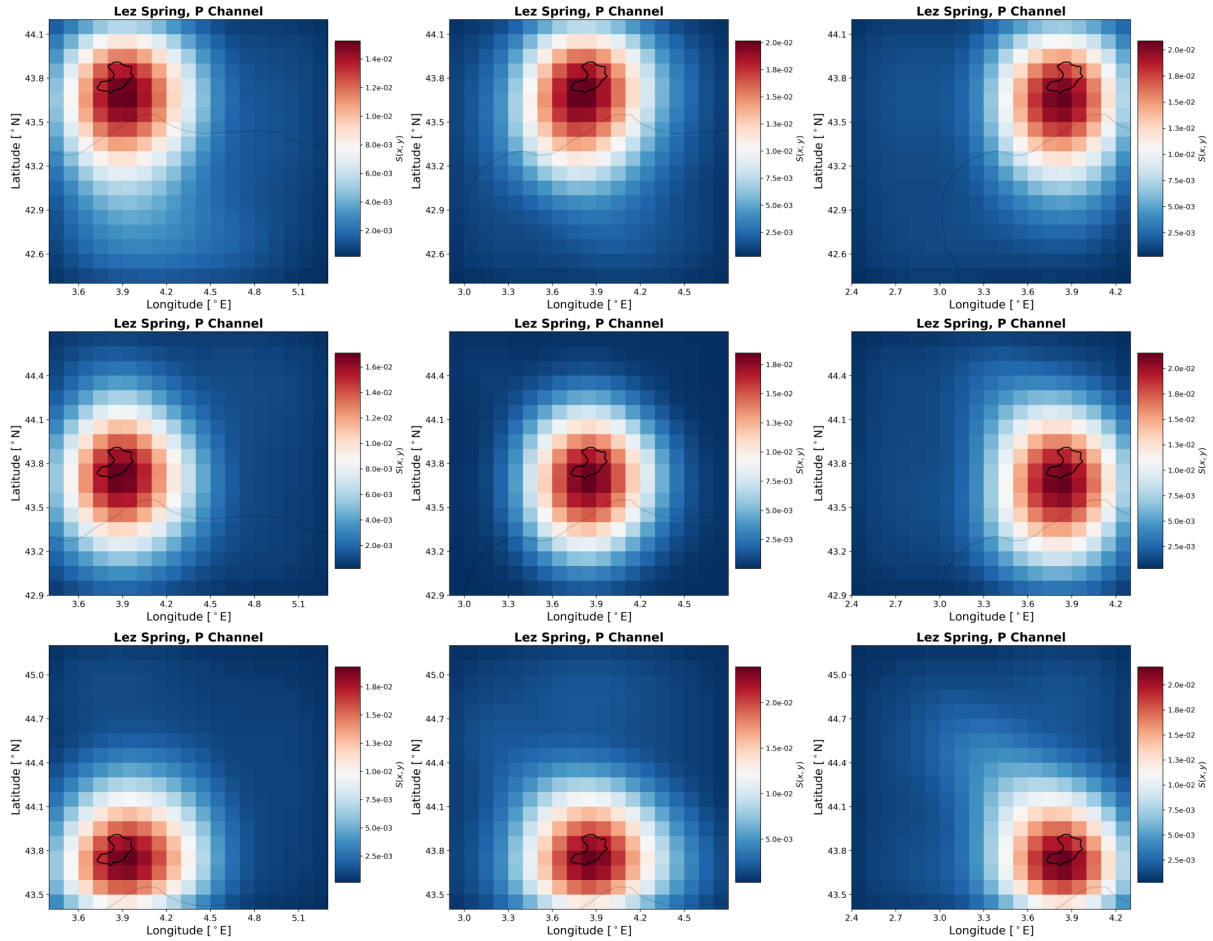
Appendix C: Heatmaps

Figure C1. Spatial input sensitivity heatmaps for Aubach spring based on ERA5-Land gridded data.

Figure C2. P-channel heatmaps based on ERA5-Land gridded data for Aubach spring with shifted area of the spatial input data frame in relation to the catchment position.

Figure C3. P-channel heatmaps based on E-OBS gridded data for Lez spring with shifted area of the spatial input data frame in relation to the catchment position.

Appendix D: Model Overview

Table D1. Model parameter summary table.

Optimized Hyperparamaters	Aubach (ERA5)	Aubach (RADOLAN)	Lez	Unica
n (1DConv filter)	128	128	16	16
input seq. length	54 (hours)	162 (hours)	53 (days)	40 (days)
batch-size	64	256	32	32
Other Hyperparameters				
inital learning rate	0.001	0.001	0.001	0.001
training epochs	100	100	100	100
early stopping patience	12	8	12	12
Model Summaries				
total parameters	708,353	1,502,849	358,977	384,017
trainable par.	708,097	1,502,593	358,945	383,985
non-trainable par.	256	256	32	32

Author contributions. AW, TL and NG conceptualized the study, AW and TL developed the methodology and software code, and validated the results. AW performed the experiments, and investigated and visualized the results. GC and ZC performed formal analysis, NR and GC contributed to data curation activities. AW wrote the original paper draft with contributions from GC and NR. All authors contributed to interpretation of the results, and review and editing of the paper draft. TL and NG supervised the work.

Competing interests. The authors declare that they have no conflict of interest.

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