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Modeling groundwater and surface water interaction: an overview of current status and future challenges

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Abstract

The interaction between surface water and groundwater constitutes a critical process to understand the quantitative and qualitative regime of dependent hydrosystems. A multi-scale approach combining cross-disciplinary techniques can considerably reduce uncertainties and provide an optimal understanding of groundwater and surface water exchanges. The simulation process constitutes the most effective tool for such analysis; however, its implementation requires a variety of data, a detailed analysis of the hydrosystem, and time to finalize a reliable solution. The results of the simulation process contribute to the raising of awareness for water protection and the application of better management strategies. Knowledge of models' parameters has great importance to ensure reliable results in the modeling process. In this study, a literature overview of modeling applications in groundwater – surface water interaction is provided. In this context, a comprehensive and holistic approach to groundwater and surface water simulation codes is here presented; results, case studies, and future challenges are also discussed. The main finding of the analysis highlights uncertainties and gaps in the modeling process due to the lack of high frequency and depth dependent field measurements. In many studies, authors underestimate the importance of the hydrogeological regime, and the discretization of hydraulic parameters is often lumped in a simplified manner. The modeling ethics in terms of data transparency and openness should be widely considered to improve the modeling results. The current study contributes to overcome common weaknesses of model applications, fulfils gaps in the existing literature, and highlights the importance of the modeling process in planning sustainable management of water resources.

Key words: MODFLOW, SWAT, overexploitation, groundwater depletion, stream.

1 Introduction

Groundwater (GW) constitutes a valuable source for human society's development and sustainability. In the framework of the Sustainable Development Goals (SDGs) to be achieved by 2030 (United Nations, 2015), one of the top-flight topics states the necessity of sustainable management of water and sanitation globally. In particular, the sixth SDG asserts the primary importance of protecting and restoring water-related ecosystems. Hence, the preservation of GW quality and quantity constitutes an emerging priority worldwide. GW as part of the water cycle is dynamically interconnected with surface water (SW) bodies such as rivers, streams, lakes, and wetlands (Winter, 1999). The interconnection is bidirectional depending on the hydrogeological regime and climatological conditions. For instance, in some cases, rivers recharge GW during the wet period, while during the dry period GW contributes to the preservation of river baseflow (Mukherjee et al., 2018). In the last decades, human activities have altered the natural balance between SW and GW. Construction of dams upstream decreased river discharge downstream, and thus the river seepage toward GW in lowlands (Fazel et al., 2017; Marcinkowski and Grygoruk, 2017). On the other hand, overexploitation of GW in lowlands due to poor water resources management leads to piezometric decline (Custodio, 2002), and consequently, river baseflow is diminished during dry seasons. Since GW abstraction to meet water demands cannot be eliminated (Herms et al., 2021a), recent studies have focused on the quantification of the components influencing GW and SW interaction. The understanding of such hydrosystems requires the evaluation of both SW and GW components giving prominence to their dynamic interaction. Obviously, the large number of parameters that influence their interaction requires specified tools and technics with the ability to: a) analyse large datasets, b) couple both hydrodynamic and hydrochemical data, and c) provide comprehensive outputs such as graphs and maps.

The natural recharge of GW is related to climatic drivers, temporal and spatial variability of runoff events, hydrogeological conditions, and morphology of the area (Sophocleous, 1991; Arnold et al., 2000). Water is stored in aquifers and enriched by minerals and trace elements in a state of permanent underground flow, while changes in the chemical elements of water are influenced by native (geological formations) and exogenous factors which are often related with anthropic activities (Herms et al., 2021b). Thus, the movements of water in space and time can determine the alteration of its chemical composition and consequently, its quality degradation (Alley et al., 2002). The recharge and discharge characteristics of aquifers are affected by excessive water consumption in urban and agricultural areas, where the lack of water management strategies often results in the water table falling over the years (Bournaris et al. 2015, Kapetas et al. 2019). GW depletion is thus caused both by overexploitation and reduction of natural recharge due to climate variability. This phenomenon contributes also to water quality degradation and its reversion is difficult and time-consuming (Gleeson et al., 2010; Sapriza-Azuri et al., 2015). The absence of sustainable water management practices causes the slow recovery of aquifers while climate change aggravates this condition (Aeschbach-Hertig and Gleeson, 2012) due to the reduced rainfall in many regions, the increased frequency of flooding, and the rising temperatures which increase evapotranspiration. For instance, the mismanagement of irrigation systems in combination with scarce precipitation in arid and semi-arid regions can potentially lead to severe drought, water scarcity, and an increasing pumping cost (Pereira et al., 2002; Kløve et al., 2014). Thus, the aquifers' recharge mechanisms and their connection with human activities (such as industrial and agricultural activities) need to be spatiotemporally quantified to establish a robust water resources management (Foster and Chilton, 2003; Vaux, 2011). In fact, the sustainability and integrated management of GW are of utmost importance to ensure water supply for human activities as well as to protect the quantitative and qualitative regime of SW.

SW is inextricably connected to GW although their exchanges show great spatial and temporal heterogeneity in the hyporheic zone, where the two systems interact (Krause et al., 2011). The external factors affect both GW and SW, although the quality and quantity degradation results in different times in each system (Sophocleous, 2002). Quality degradation and quantity depletion are even caused by human activities (Peters and Meybeck, 2000), such as: a) water contamination (e.g. sewage and fertilizers), b) land-use practices (e.g. agricultural activities and road construction), and c) hydroengineering (e.g. dams). These activities in conjunction with the global climate variability and local characteristics of the watershed (size, topography, and aquifer geometry) can potentially aggravate the phenomena of intermittent streams and the reduction of aquifer storage due to the water table drawdown (Brunke and Gonser, 1997; Bertrand et al., 2014). The climate variability directly influences SW bodies in contrast to GW which shows higher resilience to climatic stresses (Green et al., 2011) and human interferences, such as irrigation (Santos et al., 2014). Moreover, through vertical movements from the surface to the aquifers, water is filtered through the geological formations, and pollutants accumulated during surface runoff may be degraded and/or adsorbed on aquifer materials (Zhou et al., 2014). Therefore, GW is less vulnerable to quality degradation due to external factors compared to SW (Foster and Chilton, 2003). Hence, the lithology and hydraulic characteristics of an aquifer are critical factors of GW flow and contaminants' movement (Alley et al., 2002), especially in karst aquifers (Hartmann et al., 2021).

The increasing degradation of freshwater quality and quantity has been clearly documented over the last years. All strategies to mitigate this multi-component phenomenon involve simulation of both SW and GW systems. A careful study of the dynamic interaction between SW and GW can provide important guidelines for sound exploitation of water resources and the prevention of further quality and quantity degradation. However, the research on SW-GW interaction is a great challenge. For a long time, SW and GW domains had been defined as separate entities. Only relatively recently, researchers have quantitatively analysed the water movements between surface and deeper lithological layers focusing on hyporheic exchange flow (Kalbus et al., 2006). Various methods were established to analyze and manage quality and/or quantity exchanges between SW and GW such as: isotopes analysis and elements' speciation (Kazakis et al., 2015; Jasechko et al., 2017; Caschetto et al., 2017; Parlov et al., 2019), statistical analysis and modeling (Hu et al., 2007; Triana et al., 2010; Mastrocicco et al., 2014; Colombani et al., 2016; Bui et al., 2020), thermal approach (Constantz et al., 2002; Duque et al., 2010; Zhou et al., 2018), and geophysical techniques such as electrical resistivity tomography and airborne electromagnetic surveys (Boucher et al., 2009; Kazakis et al., 2016; McLachlan et al., 2017;). All these methodological approaches contribute to the management and preservation of SW and GW systems.

According to Mercer and Faust (1980a), the models are useful in identification, interpretation, and prediction studies. Models are divided into physical (laboratory) and mathematical models. Physical models include columns and tanks experiments in which natural processes are directly measured and then scaled to larger media. On the other hand, mathematical models are categorized into data-driven and process-based models (Anderson et al., 2015). Process-based models might be stochastic or deterministic. The process-based deterministic models provide more interest in the topic of SW-GW interaction because they can make acceptable forecasts under data scarcity and lie outside the range of stresses in the historical records (e.g., climate change) (Anderson et al., 2015). In literature, there are several classifications of models (Jajarmizadeh et al., 2012). Process-based models (P-b models) according to the analysis of Anderson et al. (2015) focuses on flow dynamics and transport. In the first category, the modeling focuses on the quantification of recharge, water budget, water flow, and discharge to SW bodies (Hantush, 2005;

Houben et al., 2018), while in the second category the modeling focuses on pollutant transport (Kazakis et al., 2020), including advection, dispersion, diffusion, and reaction within the hydro systems (Anderson, 2005). The current study is centred on the first category of P-b models. Moreover, in this overview we did not focus on lumped models which are used to understand the straightforward and complex hydrological process in porous, karst and fractured rock aquifers (Samper et al., 2015; Jódar et al., 2018; Herms et al., 2019). Lump models can contribute to the understanding of the interaction between surface water and groundwater as well as to the function and management of the karst aquifer (Kazakis et al., 2018). A future step of this article is to analyze the application of lump models in the topic of SW-GW interaction and compare it with regional-scale simulation.

Nonetheless, modeling requires data affluence and is time-consuming to provide reliable results. In literature, many studies have tried to simulate SW-GW interaction under data scarcity increasing the uncertainty of the application. Such applications could provide more accurate results by choosing the optimal code and software to be used. In some studies, authors provide models and advances in GW-SW interaction (Winter, 1995; Bobba, 2012; Barthel and Banzhaf, 2016).

In this study, an overview of existing studies using simulation approaches for SW-GW interaction is provided. Additionally, the main factor is stream water bodies. Wetlands are flooded by water permanently or seasonally. On the other hand, lakes are filled with water and are fed/drained by rivers. Nowadays, artificial lakes are one on the top research topics due to their importance in industrial and agricultural uses. Hence, this study aims to provide an overview of the available simulation codes and the applications in the existing literature to overcome future subjectivity in SW-GW simulation. Within this overview, scientific articles which are included in the Scopus database have been analysed to provide the status and the future challenges on Stream-GW quantity interaction modeling approaches.

This review can help researchers to: a) choose the optimal code and software, b) compare their results with other case studies, and c) stimulate new researchers to study SW and GW in an interdisciplinary manner.

2 Groundwater-surface water interaction modeling

2.1 Groundwater – Surface water Models

The aim of numerical modeling is to provide a quantification of various processes within the analysed system along with uncertainties related to parameters estimates. Models can be used for the prediction of future alterations of an aquatic system (such as the water table fluctuations in irrigated areas), and the interpretation of water exchange between SW and GW in the hyporheic zone. In literature, the modeling applications are usually focused on GW or SW neglecting the dynamical interaction between them. In some cases, GW or SW are considered as a single parameter (e.g. infiltration/exfiltration) and described in sub-packages of the model. For instance, MODFLOW comprises the stream-flow routing (SFR2), river (RIV), and stream (STR2) packages for the simulation of SW in the basin. Examples of modeling applications focusing on GW interaction with SW include: lakes (Lin et al., 2018), wetlands (Frei et al., 2009), saline intrusion (Kazakis, 2018; De Filippis et al., 2019), Aquifer Storage and Recovery via MODFLOW (Sheng, 2005; Niazi et al., 2014; Missimer et al., 2015).

A key step before the simulation process is the definition of the stress period. The user defines the starting and ending time of the stress period as well as the time step multiplier. The total period is divided into recharging periods (stress periods) and according to the type of charging of the model, each period is divided into time steps. The steady-state stress period is used to set the initial conditions before the beginning of the transient simulation. Another major factor in the simulation process is the set of boundary conditions to apply. They refer to the inflow and outflow of water fluxes through the model boundaries. Specifically, the boundary conditions refer to the hydraulic and lithological conditions of the aquifer boundaries. Neumann condition is one of the common boundary conditions for groundwater flow. This term refers to the connection between the porous media and the impermeable layer in terms of a prescribed flow between them. Additionally, the Cauchy condition corresponds to the head-dependent flow limit cases where the aquifer is connected to an adjacent one.

For the conceptualization of a hydrosystem including SW-GW interaction the following data and measurements are essential:

a) GW level measurement: according to GW level measurements, the definition of the initial aquifer conditions and the model calibration can be achieved. This term refers to time series of GW levels measured at many observation points (e.g., piezometers and/or wells) that should be distributed ideally throughout the aquifer. The number of measurements is depended on the problem to be solved.

b) Lithological profiles: from the lithological profiles the aquifer thickness and its structure can be determined. Additionally, the material of the saturated and unsaturated zones can be defined. In the case that pumping tests are not available the hydraulic data can be determined according to the material of the provided lithological profiles using empirical formulas like Kozeny-Carman for unconsolidated sediments (Carrier, 2003) or range of literature values (Anderson et al., 2015).

c) Pumping/slug tests: the hydraulic data of an aquifer are essential for numerical modeling. Pumping/slug tests can provide the hydraulic conductivity, transmissivity, and storativity of the aquifer.

d) Streamflow measurement: streamflow measurements can provide essential information about the hydrodynamic characteristics of SW bodies and their response to meteorological conditions. In general, the hydrodynamic response of the river streamflow depends on both the meteorological conditions (i.e., precipitation) and the piezometric level of the underlying aquifer.

e) Meteorological data: the measurements of parameters such as precipitation, temperature (max, min), evapotranspiration, and wind speed with a daily time step are essential to estimate infiltration and run-off which in turn may lead to GW recharge and SW flow, respectively. This information is important in defining the water budget and therefore the SW-GW interactions.

f) Water quality measurements: the physicochemical and hydrochemical data such as electrical conductivity, pH, temperature, major ions, and trace elements are essential to model hydrochemical processes, pollution transport, and predict future trends of GW quality.

The Geographical Information Systems (GIS) are useful to create files with the spatial distribution of parameters such as the bottom of the aquifer and surface elevation. Large time series of meteorological data can be analyzed with several software (excel, spss) or programming languages (R, Python) and prepared for the modeling process. The consistent analysis of all the above data led to the conceptualization of the hydrosystem, defining the main terms of the water balance, and the geometry of the aquifer including boundaries, the recharge and discharge zones, and other important features such as springs and wells.

2.1.1 Groundwater

GW models can be divided into physical (laboratory) models and mathematical models, further divided into analytical and numerical models. Physical models include laboratory tanks with soil materials for the simulation of porous layers to measure GW head and flow. The analytical models provide exact mathematical solutions to simple GW flow and solute transport problems. These solutions may be used as benchmark problems for validating the solutions obtained with numerical models, which in turn are used for simulating complex hydrogeological phenomena, like the impact of water injection on the regional GW flow regime (Mercer and Faust, 1980b; Anderson et al., 2015). The application of a numerical model involves:

(i) build of a consistent conceptual model,

(ii) data collection (such as meteorological, morphological, and field data),

(iii) data preparation including the determination of boundaries in the studied area,

(iv) initial simulation and calibration of the model,

(v) simulation of GW and predictions.

The necessary parameters and input data for GW modeling are the following:

1) Hydraulic conductivity: the conductivity tensor (Kx, Ky, Kz) depends on the type of matrix in the modelled domain.
2) Aquifer layers: separation of aquifer layers according to their characteristics.
3) Transmissivity and storage coefficient: aquifer capacity to release water is given by transmissivity values. The storage coefficient is the quantity that relates the change in fluid potential (i.e., hydraulic head) in the aquifer to the change in the amount of water stored in the aquifer. Transmissivity can be

determined from pumping tests using analytical solutions like Theis Cooper and Jacobs providing the ability of the aquifer to transmit water through its saturated thickness.

4) Pumping rates: the pumping rate for a specific time period is used for the transient simulation.
5) Water levels: definition of the phreatic zone and its variations over the recording period.
6) Boundary conditions: exchanges of flow between the model domain and the external system. Separated into Flow boundary conditions (river, stream, evapotranspiration boundary conditions) and transport boundary conditions (recharge concentration boundary conditions). Separation of flow and no flow areas.

GW modeling requires several steps, from basic geological research and classical hydrogeological data to advanced elaboration of the spatiotemporal distribution of hydrological and hydrogeological data. The conceptualization of the aquifer is strongly dependent on the quantity and quality of the data as well as the experience of the researcher (Guymon and Hromadka II, 1985; Anderson et al., 2015).

Many software has been developed for different pollutants and aquifer types however the selection of the best model for each situation is crucial and depends on (i) the physical characteristics of the hydrogeological system, and (ii) the hydrochemical process to be assessed. As valid examples of GW modeling tools, SEAWAT is used for the simulation of seawater intrusion in coastal aquifers (Mastrocicco et al., 2012; Dunlop et al., 2019), and FEMWATER-LHS is used for saturated–unsaturated porous media (Hardyanto and Merkel, 2007).

2.1.2 Surface water

SW bodies include lakes, wetlands, and streams. All these systems interact differently with GW and determine the local hydrochemical regime. River-torrents influence both at local and regional scales GW quality and reserves. This article is centred on SW-GW interaction due to the high dynamics of both components and the scale of their interaction at the hydrogeological basin scale.

Various input data are used to divide the watershed into multiple sub-watersheds that are then further subdivided into hydrologic response units (HRUs) that consist of all those portions of a territory characterized by unique land use, morphological, and soil attributes combination (Neitsch et al., 2000).

A basic application of a SW numerical model involves the collection of the following data:

a) Elevation: a digital elevation model (DEM) is used to delineate the watershed boundary, streamflow direction, and morphological conditions for the slope definition into classes.

b) Land cover: land use data conducted by agricultural, residential, and industrial activities, water, wetlands, and natural vegetation data. Crop data such as plant growth-harvest-burn, management (plowing, crop rotation), and percentage of vegetation cover are important input data to quantify water erosion and evapotranspiration while fertilizer details (amount and type of fertilizer) can be applied for chemical simulation as nitrates and phosphate.

c) Soil: the spatial distribution of soil physical and chemical characteristics defines the soil parameters in the watershed. The soil map can be conducted according to soil datasets from world data centres. Soil properties such as texture, structure, and porosity determine the runoff and infiltration rate.

d) Meteorological data: the measurements of parameters such as precipitation, temperature (max, min), solar radiation, wind speed, and relative humidity in a daily time step are essential to calculate the infiltration of GW and consequently GW balance.

e) Water quality data: stream and/or watershed quality data (nutrients, pesticides, algae, bacteria, organic chemicals, heavy metals) impact the water quality conditions of the area.

Usually, daily or monthly average measurements of SW flow and quality are sufficient, while hourly measurements can provide more information for the response of the hydrosystem. The simulation begins with a warm-up process that uses a small part of the data set for the model to reach an optimal state, where internal stores (e.g., soil moisture) move from the estimated initial condition to an optimal state. The higher the warm-up period the better results will provide the simulation of the stream flow.

The model calibration is usually implemented by using daily or monthly input data such as stream flow, evapotranspiration, and hydrochemical parameters. It is essential to determine a part of the data set for the calibration process. Usually, the calibration data corresponds over 50% of the entire data set. Moreover, it is important to split the data into two sub-datasets that can be comparable in terms of meteorological patterns. The calibration process can be obtained automatically from the software as well as manually from the end user using a trial-and-error approach. Afterwards the calibration, a short period of the data set is chosen to validate the calibration process. It is recommended the calibration period be different from the verification period. In literature, the verification process is also referred to as validation. To evaluate the model performance several statistical coefficients are available such as: the coefficient of determination (R^2), Nash–Sutcliffe efficiency (NSE; Nash and Sutcliffe, 1970), and percent bias (PBIAS; Gupta et al., 1999). A list of performance values is suggested by Moriasi et al. (2007).

The exchanges of water between SW and GW are variable from the headwaters to the lowlands of a hydrological basin. The changes in morphology, soil texture, and land use are the drivers of the streamflow variability. Due to this complexity, researchers neglect the more complex process of SW-GW interaction and simplify the input and/or output of GW to SW (Saha et al., 2017).

2.2 Data sources and availability

Modeling process requires hyper parameterization of the GW-SW system to achieve simulations with a high degree of reliability. Obviously, data availability might constitute a limiting factor for the modeling. This drawback can often limit the application of numerical and physically based models mainly in small areas or basins. Obviously, at regional or national scales the modeling process is more difficult even with high data availability. In recent years, the applicability of these models (GW and SW) has greatly increased due to the possibility to use an increasing number of available global and regional datasets. Several "Open data" and "Global model products" containing an enormous amount of useful environmental data have recently become available and in conjunction with the development of remotely sensed data represent a reasonable starting point for building any type of water model. Specifically, all morphological features such as slope, watershed boundary, and surface flow direction can be easily obtained from processing DEM products through the spatial analyst in GIS environment. One of the most widely used products is the MERIT DEM, which is an unbiased global map with ~90 m resolution of terrain elevation. It was developed using existing spatial DEMs such as SRTM3 v2.1 and AW3D-30m v1, removing multiple error components such as absolute bias, stripe noise, speckle noise, and tree height bias (Yamazaki et al., 2017). In any case, a regional or national DEM with finer resolution could also be obtained from LiDAR products or spatial interpolation of points elevation. Spatial discretization of soil properties such as hydraulic conductivity, texture (% sand, silt, and clay), porosity, organic matter, and bulk density, in addition to defining soil quality and infiltration tendency, can greatly influence modeling results, especially in the SW (Busico et al., 2021). A worldwide distribution of these soil characteristics is made available by the Harmonized World Soil database (FAO, 2012). In addition, more than 196,000 soil columns are available from the World Soil Information Service "WOSIS" (Batjes et al., 2020). This data set includes standardized soil data suitable for soil mapping and earth system modeling. Hydrological modeling is also sensitive to climate data scarcity. Hence, many databases have been established to provide high-resolution meteorological data. The Climate Forecast System Reanalysis (CFSR) (Saha et al., 2014) was established to provide 36 years of global-scale (historical) meteorological data at sub-1° resolution. In addition, the CORDEX initiative of the World Climate Research Program (www.euro-cordex.net) allows the collection of continental climate data for both historical and future scenarios that are abundantly used in water modeling (Busico et al., 2021; Colombani et al., 2021; Joseph et al., 2018; Furusho-Percot et al., 2019). Subsurface input data such as porosity and hydraulic conductivity are usually obtained through permeability tests, which is time consuming and costly. An alternative is the GLobal HYdrogeology MaPS (GLHYMPS) of permeability and porosity (version 2.0) (Huscroft et al., 2018). Continental representation of land cover spatialization and change trends are made available by the Copernicus Land

Monitoring System with the Corine Land Cover (CLC) product from 1990 to 2018. A multi-parameter calibration is often mandatory to obtain good results. The availability and use of adequate data for model calibration and validation is still the main factor influencing the definition of modeling performance. For the calibration/validation of surface models several researchers have evaluated the suitability of the products "Moderate Resolution Imaging Spectroradiometer (MODIS), with remarkable results. Remotely sensed data of evapotranspiration, snow cover, soil water content, and normalized vegetation index (NDVI) can be downloaded using the AppEEARS interface (AppEEARS, 2021). Along with these "Open datasets" several modeling products have also been made available over the past decade. Among them, the WaterGAP v2.2d (Müller Schmied et al., 2021), and the PCR-GLOBWB v2.0 (Sutanudjaja et al., 2018) are two global hydrological models produced with the purpose of quantifying human use of GW and SW along with water flows and storage and water resources on a planetary scale by giving the ability to post-process several outputs such as spatiotemporal GW recharge and river flow volume. Their main limitation is the low spatial resolution. In this scenario of globally available data, it is worth mentioning that uncritical use of global databases can prove to be erroneous and dangerous since they can contain artifacts and incongruencies which can produce inconsistencies and uncertainties in simulation. In Table 1 are shown available data sets and the corresponding links to obtain the data.

Table 1. Available data sets for modeling parameters.

Raw Data	**Extension**	**Format**	**Source**
Soil Classification and property	World	Shapefile	http://www.fao.org/geonetwork/srv/en/metadata.show?id=14116 https://www.isric.org/explore/wosis
Digital surface model (DSM)	World	Raster	https://asterweb.jpl.nasa.gov/gdem.asp
Historical climatic data	World	Database	https://globalweather.tamu.edu/
Land Use classification	Europe	Shapefile	https://land.copernicus.eu/pan-european/corine-land-cov
Climate Projections	World	Database	https://esgf-data.dkrz.de/search/esgf-dkrz/
Rock permeability and porosity	World	Shapefile/Vectorial	https://dataverse.scholarsportal.info/dataset.xhtml?persistentId=doi%3A10.5683/SP2/TTJNIU
MODIS products	World	Raster	https://lpdaacsvc.cr.usgs.gov/appeears/task/point
Historical climatic data	World	Raster	https://apps.ecmwf.int/datasets

2.3 Available software

GW and SW are interconnected components of the hydrologic cycle and are both affected by external factors such as climate change, geological formations, and anthropogenic activities (Sophocleous, 2002). Although SW and GW can be analysed as separated components, the approach of an overall analysis of SW-GW interactions can provide optimal data for better water management applications. In the case of Stream-GW interconnection, streamflow is directly influenced by climate variability and change and consequently GW recharge worldwide (Zhang et al., 2007; Guermazi et al., 2019). In this section, the available software to model Stream-GW interaction is presented and applications for each software in the available literature is given.

The understanding of water horizontal and vertical exchanges between the surface and subsurface systems is crucial and maybe the most difficult part of the modeling process. Thus, a thorough approach is required to handle the challenges of implementing integrated models of saturated-unsaturated GW and SW sectors. This innovative conjunction of dynamic simulation models is also able to simulate the future trends of GW quality and quantity under climate and land use land cover changes. Consequently, three-dimensional models can depict thoroughly the water flow in comparison to one-dimensional and two-dimensional models (Sophocleous et al., 1995). Modeling of Stream-GW interaction is time consuming due to a large number of data and software demands. However, such models are available rendering such modeling feasible. According to the literature review, SWAT-MODFLOW, GSFLOW, MIKE SHE, and HydroGeoSphere are the most common models for Stream-GW simulation analysis (Figure 1). The most widely used is MODFLOW for GW flow simulation, while SWAT is the dominant one for stream flow simulation. The overview of articles within the topic of numerical modeling of SW-GW interaction shows an increasing use of numerical models for the simulation of SW-GW interaction and a constant use of SWAT-MODFLOW as well as GSFLOW during the years (Table S1). The first application of SWAT-MODFLOW was published in 1999. Additionally, the initial use of GSFLOW model was observed in 2014. Moreover, most authors applied SWAT-Modflow codes in the majority of cases of forecasted simulations. Different frequency of use shows the Hydrolog-Aquifem, HydroGeoSphere and Help-Feflow-Cathy codes with limited applications on the current topic. These models after their first period of appearance present slight increase in the case study of published surveys until 2020.

The worldwide distribution of publications per used software is shown in Figure S1. The majority of case studies include case studies within the United States of America coupling SWAT and MODFLOW codes, while a significant number of case studies refer to areas of Europe.

The input data of the most used models for Stream-GW interaction are schematically shown in Table 2. Twelve main parameters have been distinguished and are analysed below:

- Climate data are used as a parameter in all the dominant software. Obviously, climate data consist of many sub parameters such as snowfall, temperature, and precipitation. These parameters are used either individually, for instance, rainfall, or conjunctively for the calculation of variables such as evapotranspiration. In some cases, models can use precipitation including snow and rainfall, or they can be used separately. For instance, snow accumulation and melting processes require the use of the snow thickness parameter, and consequently, the snow-water equivalent can be estimated. The climatic data scarcity from land-stations is often a serious problem in the simulation process. Nevertheless, in the last decades this gap is overcome by using satellite data. Additionally, the absence of parameters such as wind (speed and direction), solar radiation, and relative humidity can be overcome by using equivalent methods.

- Digital elevation model (DEM) constitutes a critical parameter for the simulation process. In some models is used for the determination of drainage network and the boundaries of the sub-watersheds. Additionally, it can be used for the calculation of infiltration.
- Land cover contributes to the spatial distribution of vegetation types to calculate transpiration values and evaporation from the leaves. Additionally contributes to the calculation of runoff and infiltration according to the land cover types. Urban drainage sites defined by low infiltration amounts, while natural vegetarian contributes to higher infiltration rates.
- Crop parameters such as crop rotations, planting, and harvest dates, irrigation, fertilizer, and pesticide application rates and timing are used for the estimation of transpiration of vegetation.
- The soil properties contribute to the estimation of surface runoff and infiltration. The soil features are described by the soil texture, water soil capacity, organic carbon content and organic matter.
- Aquifer structure and hydraulic parameters. Aquifer structure is determined by the thickness of the layer and the bottom and top elevation. The hydraulic parameters of the aquifer are hydraulic conductivity, transmissivity, storativity, and specific yield. Finally, the effective porosity of the aquifer is also used for the solving of hydraulic equations.
- Vadose zone characteristics. Similar to the aquifer, the vadose zone is described by its structure and hydraulic parameters.

- Boundary conditions of the aquifer constitute one of the most difficult requirements for the modeling process. It can be determined by using piezometric maps when the structure and hydraulic parameters of the aquifer have been determined. In some cases, initial simulations of a model are used for the determination of the boundary conditions.
- The local sources/sinks are also added to the conceptual model. Pumping data, GW level variations, and chemical analyses of a specific point (well) are used for the modeling process.

Table 2. Input parameters of most used models for SW-GW interaction.

Main Parameters	Sub-parameters
Morphology	Digital elevation model (DEM)
Climate data	Precipitation (unknown, snow, or rain)
	Temperature (minimum, maximum)
	Solar radiation
	Relative Humidity
	Wind speed
	Evaporation
Aquifer layers	Number of layers
	Thickness
	Satured-Unsatured zone
	Hydraulic conductivity
	Aquifer storage
	Transmissivity
Vadose zone	Structure
	Hydraulic conductivity
	Transmissivity
Land cover	Crop
	Urban/ Industrial
Soil	Soil texture
Stream flow	Measurements of stream flow variation

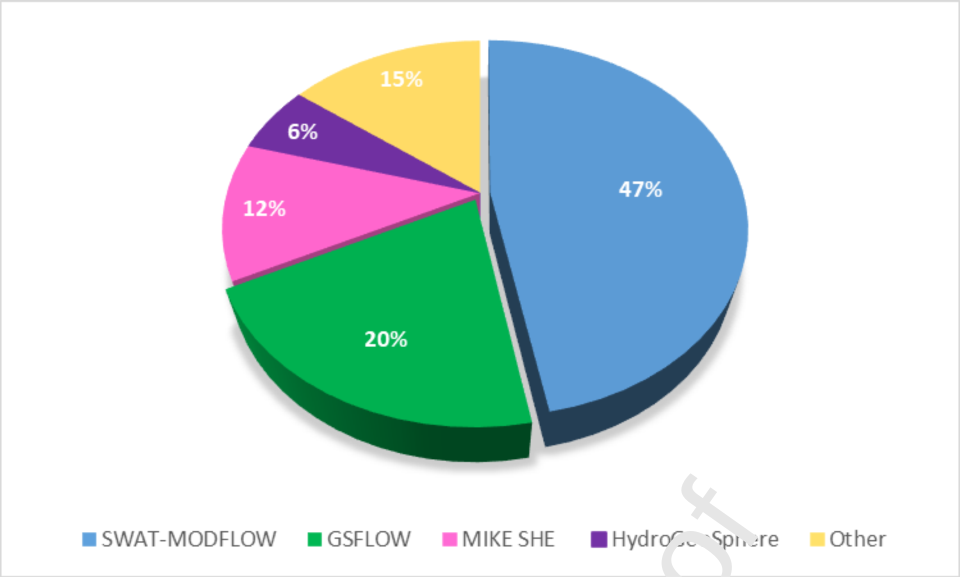

Figure 1. Most used models for SW-GW interaction from 1992 to 2020 worldwide.

2.4 Overview of modeling groundwater – surface water interaction applications

The obtained literature overview revealed that in total are 33 field sites and watershed models articles. The details are shown in Table S1, while the distribution of the case studies is presented in Figure 2. Within this section, the case studies of Stream-GW interaction categorized per software is demonstrated.

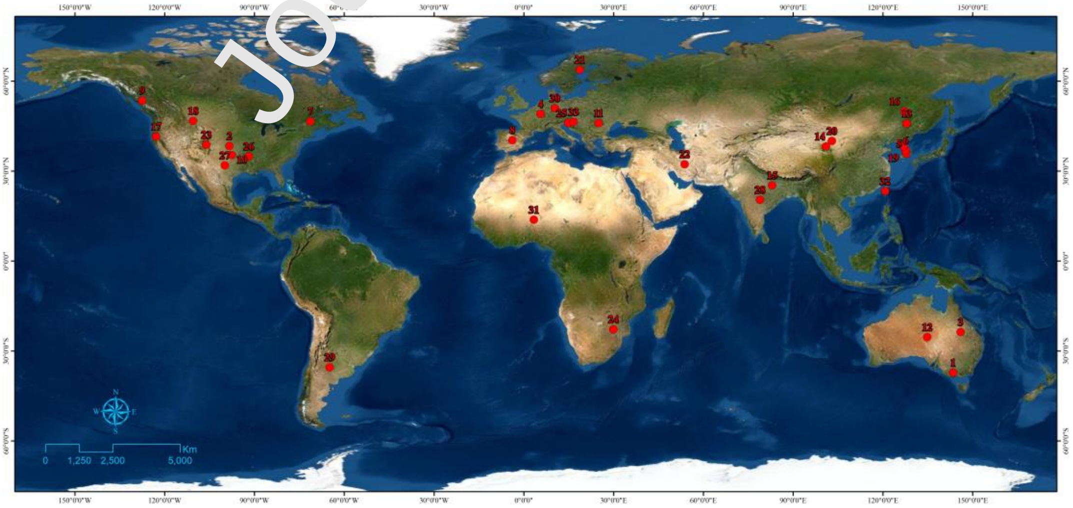

Figure 2. Spatial distribution of SW-GW interaction models' case studies worldwide.

2.4.1 SWAT and MODFLOW

The Soil and Water Assessment Tool (SWAT) and MODFLOW models are among the widely used SW and GW models, respectively. MODFLOW is a computer program that numerically solves the three-dimensional GW flow equation for a porous medium using a finite-difference method (McDonald and Harbaugh, 1988). MODFLOW has been applied in numerous studies to investigate SW-GW interaction with the River Package where Darcy's law is used to calculate the volumetric flow. MODFLOW solves both confined and unconfined flow equations to simulate the behaviour of GW flow systems under several types of natural and artificial stresses. Nonetheless, the model does not simulate surface processes such as land–atmosphere interactions, infiltration and surface runoff, plant growth, and the impacts of management practices on agricultural systems. The version MODFLOW-2005 and MODFLOW-NWT includes the simulation of saturated- unsaturated flow process, GW simulation-optimization process, irrigation process, density dependent flow process, parameter optimization process, and solute transport process. For instance, the Stream-Routing Package permits to merge or separate the flow of two or more streams (Prudic, 1989). The version 2 of the Streamflow-Routing (SFR2) Package of MODFLOW-2000 also includes the unsaturated flow beneath streams. The SFR2 helps in the simulation of the flow and storage in the unsaturated zone and the simulation of a time delay for recharging. Obviously, the current trends of the MODFLOW code are to conjunct also SW process to provide an integrated simulation. MODFLOW 6 is the latest version of the U.S. Geological Survey's modular hydrologic model. MODFLOW 6 was developed to synthesize two types of hydrologic models, the Groundwater Flow (GWF) Model and the Groundwater Transport (GWT) Model (Langevin et al., 2017).

The SWAT model (Arnold et al., 1998) simulates the land surface and vadose zone, in-stream, and soil domain processes. The Hydrologic Response Unit (HRU) includes all the hydrological data used in SWAT (such as hydraulic conductivity, storage, specific yield, and effective porosity). The model evaluates hydrological responses (water, sediment, and nutrient loss) to land use and climate changes in watersheds using a digital elevation model (DEM), soil map, land use map, climate data, crop management data, as well hydrometric and crop yield data. All the model's outputs such as runoff, evapotranspiration, aquifer recharge, sediment, and nutrient loadings from each HRU are obtained using the input of climate, soil properties, topography, vegetation, and land management practices and further summarized to obtain the sub-basins loading. SWAT includes a GW module although it cannot effectively provide the spatial distribution of data. Consequently, by exchanging characteristics of the HRUs with cells in MODFLOW in a fully coupled manner, the SWAT-MODFLOW model can estimate the amount and spatial-temporal distribution of SW-GW interactions. Additionally, the spatial resolution of the exchangeable parameters between the surface and ground systems has better distribution when the extent of the SWAT-HURs and MODFLOW-grid cells is equal. Thus, the coupled SWAT-MODFLOW model can provide a better approach to SW-GW interaction and more reliable results rather than the application of the two models separately.

Sophocleous et al. (1999) applied SWATMOD to evaluate long-term water-management strategies in the Rattlesnake Creek basin in south-central Kansas. The model runs for a 40-year historical simulation period (1955-1994), based on historical conditions of streamflow and water levels observed during the early development period from 1955 to 1980. While in the next step several hypothetical scenarios (reduction and variation in the withdrawal rates) were implemented with the calibrated model for a 40-year future simulation period (1995-2034). For the evaluation of the hydrologic impact of modifications on streamflow and water-levels based on management scenarios, the Decision Support System (DSS) module was applied. Kim et al. (2008) combined the SWAT (AVSWAT2000) and MODFLOW models to investigate the SW-GW interaction in Musimcheon Basin in Korea. The study area extends to 198 km^2, therefore 2176 pumping wells were used for the best spatially distribution of conditions. The authors used the River and Well packages of MODFLOW to calculate the quantity of GW discharge determined by hydrologic analysis from the watershed for the daily streamflow for 3 years running (2000–2002) and one year of data for the calibration period. The SWAT-MODFLOW models were also integrated by Chung et al. (2010) to compare simulated GW levels as well as the simulated watershed streamflow with the observed GW levels and Mihocheon watershed streamflow in South Korea. The packages of MODFLOW were applied for the river-aquifer interaction of 6 years (2000-2005), while the calibration years were considered between 2000 and 2001 and the validation period in 2004. The results of the simulation revealed that GW recharge constitutes 19% of the annual rainfall in the studied basin of 1,868 km^2 extension. The MODFLOW-NWT and SWAT codes were modified by Guzman et al. (2015) in Fort Cobb Reservoir experimental watershed (780 km^2) located in Oklahoma, USA. The SWAT model was calibrated for streamflow for 8 years (2005-2012) using the first year as a “warming up” period, while the SWAT-MODFLOW model was calibrated from 2010 to 2012. The case study was carried out using datasets from the Fort Cobb Reservoir experimental watershed while the authors used the SWATmf-model to refine the most sensitive parameters using available measured flow data based on needed functions. Bailey et al. (2016) applied the SWAT 2012-MODFLOW-NWT model at Sprague River watershed for 43 years (1970-2003) using daily time step. This study explored the spatio-temporal patterns of GW discharge to a river system in a semi-arid region in an area of 4,100 km^2 within the Upper Klamath Basin in Oregon, USA. The authors used the River package of MODFLOW to calculate the volumetric flow. Additionally, they converted SWAT HRUs into geographically located Disaggregated HRUs (DHRUs) and after the DHRUs into MODFLOW grid cells to exchange data between the two models. Surinaidu et al. (2016) applied the same combination of numerical models in a semi-coupled modeling framework to examine the technical feasibility of recharging the subsurface storage in the Ganges River (Ramganga Sub-basin, India). The model was calibrated from 1999 to 2005 and validated for 5 years (2006-2010). The first 2 years (1994-1995) were used as a "warm-up" period for the model. The river flow in the non-monsoon period is not sufficient to meet the needs of agriculture needs while during the monsoon floods occur. In addition, the possibility of GW recharge was evaluated in two scenarios for the forecasted period from 2010 to 2020. The first scenario follows the GW recharge patterns as in 2010, while in the second one GW recharge under increasing rainfall scenario as predicted by Inter-Governmental Panel on Climate Change (IPCC) is applied. Huo et al. (2016) used the coupled SWAT-MODFLOW model in an area of the Heihe River in China to provide a long-term integrated, quantitative water balance. First, the calibration of the model was performed from 2005 to 2008, while the first year was used as a warm-up period and the validation was performed for 5 years (2009-2013). Two future scenarios were applied, the first one for the 2020-2039 period and the second one for the 2040-2059 period. The results showed the decreasing discharge of the Heihe River for the first 20 years while in the next 20 years (2040-2059) the discharge will increase. In 2019, the coupled model was applied in a large agro-urban river basin in South Platte River

Basin, Colorado, USA from 1997 to 2012 by Aliyari et al. (2019). The model was run in the semi-arid region and tested by water table and streamflow measurements throughout the basin. Mosase et al. (2019) estimated the spatial-temporal distribution of GW recharge rates in the Limpopo River Basin, Africa. The model was calibrated and evaluated for monthly streamflow for 30 years (1984-2013), where the first 5 years were used as a warm-up simulation period. The results highlighted the disproportionate natural GW recharge compared to the water needs in the area showing the necessity of MAR application. Semiromi and Koch (2019) applied the same models in the Gharehsoo River Basin, Iran. The model was calibrated from 1988 to 2012 and tested from 1978 to 1987 with 3 years of warm up. SWAT and MODFLOW-NWT models were first calibrated individually, and afterwards an add-on recalibration of the coupled model is performed. For the connection of the two models and the data exchange, the DHRUs were used. The results showed that GW fluxes were mainly driven by streams. Wei and Bailey (2019) applied the SWAT-MODFLOW model to examine the interactions between irrigated SW-GW systems in Lower Arkansas River Valley (USA) to quantify the effects of decreasing irrigation on crop production and hydrologic responses. Bailey et al. (2020) presented a version of SWAT+ having the capability for land surface hydrology and hydrologic connections. Additionally, they used MODFLOW to simulate GW flow and SW-GW interactions within the Middle Bosque River Watershed in Texas (USA) in a basin of 470 km^2. The model was calibrated for 13 years (1993-2005) and tested for 7 years (2006-2012). The model was tested according to a set of field measurements including water table fluctuations and stream discharge. The results of both simulation approaches were similar. Sahoo and Sahoo (2020) compared the Variable Parameter McCarthy-Muskingum–enhanced hillslope storage Boussinesq (VPMM-ehsB), and the HRU based coupled SWAT–MODFLOW to study a better alternative approach for catchment decomposition between the hillslope and the HRU based on SW-GW interaction models. The methodology was applied to the Brahmani River (India) from 1986 to 1996. The calibration was performed for the first 6 years of the data set. The results reveal that the hillslope-based VPMM-ehsB model performed better than that of the SWAT-MODFLOW in predicting the average annual streamflow. Guevara-Ochoa et al. (2020) applied the coupled SWAT-MODFLOW model under climate change scenarios to quantify the spatio-temporal dynamics of water balance and GW-SW interactions for the upper creek basin of Del Azul in Buenos Aires, Argentina. The simulation was calibrated and validated in a baseline scenario for 13 years (2003–2015) and contrasted with two future scenarios of the regional climate model CCSM4 (RCP 4.5 and 8.5) for the period 2020–2050.

2.4.2 GSFLOW model

The GSFLOW model is a coupled GW and SW flow model developed by the U.S. Geological Survey (USGS) based on the integration of the USGS Precipitation-Runoff Modeling System (PRMS-V) and the USGS Modular GW Flow Model (MODFLOW-2005 and MODFLOW-NWT) relying on a simplified equation for simulation of water flow. The GSFLOW model can simulate the hydrologic processes from the plant canopy to the vadose zone in a daily time step while does not contain modules for handling hydraulic storage structures. PRMS is a module to evaluate the effects of various combinations of precipitation, climate, and land use on a watershed. (Leavesley et al., 1983). Additionally, MODFLOW simulates the recharge and discharge rates of water in porous and fractured aquifers. The two models have similar programming framework simulating flow across the land surface and within subsurface saturated and unsaturated materials coupling the 1D surface hydrology simulation and 3D GW simulation. The PRMS and MODFLOW remain separate in the integrated model while the data of PRMS are discretized into HRUs and MODFLOW data are discretized using a finite-difference grid or into HRUs. The initial version of GSFLOW does not include all capabilities of the PRMS and MODFLOW models, while the main packages used (according to the following research papers) are the Streamflow Routing package (SFR2) and Unsaturated Zone Flow package (UZF1) for the simulation of streams and vadose zone respectively. The SFR Package originally was developed for MODFLOW-2000 (Prudic et al., 2004) and was revised by Niswonger and Prudic (2005) to simulate unsaturated flow beneath streams. The package was subsequently revised for MODFLOW-2005 and then for GSFLOW to simulate kinematic-wave routing. The Streamflow-Routing Package is a modification of the River Package described by McDonald and Harbaugh (1988). The new package is designed to route flow through one or more rivers, streams, canals, or ditches in addition to computing leakage between the SW and the GW system.

Hassan et al. (2014) applied the GSFLOW model to investigate the river-GW interaction in fissured rock aquifer in the semi-arid Sardon Catchment (Spain). The model was calibrated and post-audited using 18 years of daily GW head and stream discharge data. The catchment covers an area of 80 km^2 granitic aquifer under alluvial deposit formations characterized by shallow water table conditions and relatively low storage. In this study, the vertical unsaturated flow is simulated using a kinematic wave equation and lateral unsaturated flow is neglected beneath the soil zone. The calibration of the model was performed for 16 years (1995-2010) while the first year was used as a warm up period. The results revealed that integrated hydrologic model can handle surface–groundwater interactions in a more realistic way integrating fluxes of the entire water cycle in comparison with the use of standalone models. Tian et al. (2015) coupled the GSFLOW model with hydraulic engine of the Storm Water Management Model (SWMM) in Zhangye Basin which belongs to the Heihe River basin (China). The basin covers an area of 9.097 km^2. The SWMM model enriched the simulation of 9 years (2000-2008) hourly time-step for river-GW interaction of hydraulic structures in GSFLOW model application. Different scenarios were applied on different agricultural water supply activities and water management scenarios impacts for the same simulation period. The outcome reveals the importance of water management solution implementation to overcome GW depletion in the future. Tian et al. (2016) applied the GSFLOW model in the Heihe River Basin (northwest China) with a basin extent of 90,589 km^2, to investigate water supply and address environmental issues. To analyze the complex hydrological modeling, the authors used the visualization tool IHM3D (Integrated Hydrological Modeling). The GSFLOW model was run for 13 years (2000-20012) with the first year as a "spin-up'' period and the results showed good performance of GW simulation. In 2018, the authors (Tian et al., 2018) improved their previous simulations by applying the Water Resources Allocation (WRA) module in GSFLOW to investigate the hydrological impacts of the joint operation on SW and GW reservoirs the in Heihe River Basin for the period of 2000-2012. Essaid and Caldwell (2017) used GSFLOW to investigate the SW flow, GW discharge, and the interaction of the two components as well stream temperature change in the watershed of the Smith River in Montana (USA) caused by irrigation practices. The study area covers 640 km^2, where the authors applied the model for 6 years (2005-2010) to examine the water flow movements in combination with temperature changes in the ecosystem (fish habitat). The results provided important data for the application of three scenarios of irrigation practices alterations. Joo et al. (2018) successfully implemented the same model in the Miho catchment (Korea) for 10 years (2004-2014) while the first year was used as a warm-up period. The catchment drains an area of approximately 2100 km^2 and the length of the Miho stream is approximately 97 km. The study area spans a range of different geological formations including sedimentary and crystalline rocks. The various geological formation determines the hydrogeological regime of porous and fissured rock aquifers. The climate of the study area is humid, while flood events are the major threat to human activities. The authors investigate the SW-GW interactions in combination with damping effects and water management techniques for floods and droughts. Tran et al. (2020) applied GSFLOW to analyze the SW-GW interactions considering the artificial recharge lake in Pingtung Plain (Taiwan). The authors examine the values of streamflow during the wet and dry periods. The results of 3 years simulation showed insignificant water budgets due to the small extension of the lake.

2.4.3 MIKE SHE

The MIKE SHE is an integrated hydrological model developed by the Danish Hydraulic Institute (DHI) based on the SHE (Système Hydrologique Européen) code combining components of the hydrological cycle (Refsgaard and Storm, 1995). MIKE SHE is a widely used software for fully coupled SW and GW modeling considering overland flow, interflow, base-flow, and transport of solutes.

In the 2003 version, all major hydrologic flow processes are dynamically coupled, including 2D overland flow, 1D channel flow, 3D saturated zone flow, 1D Richard's equation unsaturated zone flow, snowmelt, and evapotranspiration. MIKE SHE can be linked with MIKE 11 for the simulation of hydraulics, sediment transport and morphology, and water quality in the riverbed. MIKE 11 is a 1D river modeling system based on the complete dynamic wave formulation of the Saint Venant equations (Havnø et al., 1995). The main two modules of MIKE SHE are PP (pre- and post-processing module) and WM (water movement module) including the sub-packages of evapotranspiration (ET), unsaturated zone flow (UZ), saturated zone flow (SZ), overland and channel flow (OC), and irrigation (IR).

Voeckler et al. (2014) used MIKE SHE to investigate the potential contribution of deep GW recharge with snowmelt-dominated headwater catchment in mountainous terrain in the Okanagan Basin (British Columbia). MIKE SHE was coupled with MIKE 11 to simulate flows in the river system. The results showed a good performance between snowmelt and streamflow, in contrast with model performance for the unsaturated and the saturated zones due to the complexity of the mountainous bedrock system while the water table movements did not respond to the recorded rain events. According to the authors, the average water balance results indicate a recharge to the bedrock of 27% of the annual precipitation. Sandu and Vista (2015) applied the same simulation methodology in the Argesel River Catchment (Romania). The coupled model MIKE SHE and MIKE 11 was used to evaluate the rainfall-runoff process in the basin with an extent of 242 km^2. Two rainfall events were used for the calibration of the model for the periods 1/8/1997-12/8/1997 and 21/3/2007-26/3/2007. The parameters of drainage time constant, and hydraulic conductivity were updated in MIKE SHE after the calibration process. In MIKE 11 was calibrated the manning's coefficient for channel flow and leakage coefficient. The model then was validated for the periods between 16/8/2005-24/8/2005 and 19/10/2009-24/10/2009 by using daily step. Sterte et al. (2018) investigated the influence of catchment characteristics and freeze-thaw processes on SW-GW interactions by applying MIKE SHE in the Krycklan catchment (Sweden). The modules of MIKE SHE used in this study are overland flow, river flow, unsaturated-zone flow, saturated-zone flow, and evapotranspiration. The simulation was performed for the period from 2009 to 2014, while the validation was performed for the period 2013-2014. The model was used to examine the representing catchment hydrological functioning. Waseem et al. (2020) simulated the hydrological and hydraulic processes in the Tollense River basin (Germany) from 2010 to 2018 covering strongly varying meteorological conditions with MIKE SHE and MIKE 11. The catchment covers an area of 400 km^2 and is characterized by intensive agriculture activities. The study showed a strong influence of land use type and local meteorological conditions in the spatial distribution of water balance in the study area.

2.4.4 FEFLOW – MIKE 11

The FEFLOW (Finite Element subsurface FLOW) was created in 1979 by the Institute for Water Resources Planning and Systems Research Inc. (WASY GmbH) of Berlin, Germany, which has recently become a part of DHI Group. The model is used to simulate subsurface flow, mass and heat transport processes and it is generally used in combination with MIKE surface model for the investigation of SW-GW interaction in simple or complex geometrical configurations of hydrogeological formations. The variables for calculation of GW flow include the permeation coefficient, rate of GW recharge, the bottom elevation of the water-barrier of the phreatic aquifer, and the top elevation of the aquifer, etc.

Vrzel et al. (2019) coupled FEFLOW and WaSiM/MIKE 11 to examine the interactions between precipitation, river water, and GW under different future climate scenarios. The research area was a part of the Sava River (Ljubljansko polje, Slovenia). The authors used the FEFLOW 3D while MIKE 11 and WaSiM for river flow and percolation of local precipitation. In the first stage of simulation GW and precipitation daily data were calibrated and simulated, for the second stage the three Regional Climate Models (RCMs) for 2036-2065 were used. The results from the combined climate projection and simulation models showed that the aquifer is more susceptible to climate variations in groundwater abstraction zones.

2.4.5 MODHMS

MODHMS is a successor to MODFLOW-SURFACT and is similarly based on MODFLOW-88 (McDonald and Harbaugh, 1983). MODHMS includes the channel flow package which solves the diffusion wave approximation of the one-dimensional Saint Venant equation. The 3-D variably saturated flow via stream leakage and connection with GW can be simulated by using the Richards equation.

Werner et al. (2006) investigated the influence of SW-GW interaction on Sandy Creek River in Australia by applying MODHMS including the Streamflow Routing (STR) package. The authors used a long historical rainfall record for the simulation scenario. The MODHMS overland flow package (OLF1) was used to solve the diffusion wave approximation of the vertically- averaged Saint Venant equations for areal overland. In the second stage of the research, the model has been tested using stream depletion analysis and radon isotope tracer sampling. Within this study, was quantified SW-GW interaction and compared with baseline flow of streams. The baseline flow was estimated by using three hydrography separation methods. These methods were not able to reflect the time dynamics of this exchange for Sandy Creek basin due to the influxes of short-term release from stream bank and instream storage.

2.4.6 HYDROLOG - AQUIFEM-N

The Monash Rainfall-Runoff Model, HYDROLOG (Porter and McMahon, 1976) is used to represent the surface hydrological processes while the multi-Layered Finite-Element Aquifer Flow Model (AQUIFEM-N) is applied to model the GW flow (Townley, 1987). AQUIFEM-N is a quasi-three-dimensional model based on the finite-element method with linear triangular elements. Aquifer properties include the aquifer bottom elevation, aquifer thickness, hydraulic conductivities, or transmissivities (including arbitrary orientation to any anisotropy), specific yield, aquifer storage coefficient and leakage coefficient through an adjacent aquitard. Chiew et al. (1992) coupled the daily version of the Monash Rainfall-Runoff Model, HYDROLOG and AQUIFEM-N in Campaspe River Basin (north-central Victoria). The simulation covered 7 years of simulation (1981-1987). The integrated model was calibrated with streamflow and GW potentiometric head data, while recharge was estimated as an output from the calibrated model. The results provided the spatial and temporal distribution of regional recharge rates resulting from rainfall and irrigation water.

2.4.7 HELP- FEFLOW- CATHY

The Hydrologic Evaluation of Landfill Performance (HELP) model (Schroeder et al., 1994) was first designed as an assessment tool for infiltration in landfills by the U.S. Environmental Protection Agency. In the last decades it has also been used as a two-dimensional hydrologic model for the simulation of SW-GW interaction. The model estimates daily actual evapotranspiration (ET), surface and subsurface runoff, and vertical drainage for a soil column by performing a water balance analysis. Its input parameters are of three types: climate data, surface data, and soil physical properties.

The Finite-Element subsurface (FEFLOW) model (Diersch, 1998) is available for simulation of density-dependent GW flow. The model can apply predict rates of infiltration/aquifer recharge due to precipitation, storm water retention ponds or artificial aquifer recharge schemes as well can determine the spatial and temporal distribution of GW heads.

CATHY (CATchment HYdrology) is a coupled model system of surface and subsurface water flow at the catchment scale. CATHY combines a finite element solver for the three-dimensional Richards equation describing flow in variably saturated porous media while a path-based one-dimensional diffusion wave equation is used for hillslope (rivulet) and stream channel flow, with a different parameterization for these two elements of surface runoff (Paniconi and Wood, 1993; Paniconi and Putti, 1994). In general, outputs from the CATHY model include overland fluxes, subsurface pressure head, moisture content values, and GW velocities. The main input data for CATHY are summarized as follow: DEM, terrain, rivulet, and channel analysis parameters; soil properties, saturated hydraulic conductivity, specific storage and porosity, atmospheric fluxes, and boundary conditions.

Guay et al. (2013) applied two different modeling approaches in a part of the Allen Creek stream catchment (Quebec, Canada). First, the authors applied the HELP infiltration code to calculate evapotranspiration, runoff, and recharge rates in response to atmospheric forcing at the land surface in combination with the 3D finite-element GW flow software FEFLOW. In the second approach, CATHY numerical model was used to couple a diffusion wave surface routing equation to a 3D Richards equation representation of the saturated subsurface flow variably. Both approaches provided reasonable inferences with quite different results on a detailed scale of the comparable models.

2.4.8 WetSpass-M - MODFLOW

The modified WetSpass-M (Water and Energy Transfer between Soil, Plants and Atmosphere under quasi steady state) model is a raster-based water balance model that partitions precipitation into interception, surface runoff, evapotranspiration, and recharge for each grid cell (Batelaan and De Smedt, 2001) based on WetSpa. The grid cell water balance for each time step includes interception, surface runoff, evapotranspiration, and recharge values. Salem et al. (2020) applied WetSpass-M and MODFLOW to investigate the analysis of regional Drava River and GW flow systems (between Hungary and Croatia). The authors tried to analyze the restoration of natural reservoirs (abandoned paleochannels) as management aquifer recharge (MAR) solutions. The simulation highlighted the strong interconnection between the MAR reservoir and GW giving a promising solution against water shortage problems.

2.4.9 HydroGeoSphere

HydroGeoSphere (HGS) has been developed by extending the FRAC3DVS code to accommodate surface and subsurface flow and solute transport (Therrien et al., 2009). The HGS simulates water flow in a fully integrated model. SW-GW interaction is simulated by using a 2D and the 3D form of Richards' equation for variably saturated flow.

Batlle-Aguilar et al. (2015) used and calibrate the HydroGeoSphere model with pilot points using different combinations of GW heads and infiltration volume data at Pedler Creek catchment in Australia. The main concept of this research is focused on the investigation of the SW-GW connectedness and infiltration rates under natural flow events. The results highlighted the lateral connection between the stream and aquifer through a high permeable formation in the streambank. Boubacar et al. (2020) used the same model to study GW-SW interaction in geologically complex fractured and sedimentary aquifers in a part of the Niger River in Africa. The authors provided a method for reducing the calibration effort of large-scale hydrologic models.

2.4.10 WaSiM-ETH-I - MODFLOW

The grid-based Water Flow and Balance Simulation Model (WaSiM) is a well-established tool for investigating the spatial and temporal variability of hydrological processes in river basins, however, the last publications of the current model are up to 2013.

Krause et al. (2007) applied a combination of WaSiM-ETH-I and MODFLOW models to investigate the soil and land-cover characteristics for the quantification of exchange fluxes across the SW-GW in Havel River basin, Germany. The authors provide an extensive study of the large (19,800 ha) floodplain of the Lower Havel River that have involved the development of the Integrated Modelling of Water Balance and Nutrient Dynamics (IWAN) modelling system.

Considering the literature overview, it is necessary to examine the individual parts and process of the involved hydrosystem in the GW-SW interaction concept. Stream, aquifer, vadose zone and hyporheic zone characteristics are the main involved parts.

External factors such as temperature and precipitation should be carefully evaluated due to their variability in space and time (Krause et al., 2009). The sources of uncertainty have been highlighted in many referred studies and thus researchers should address them (Goderniaux et al., 2009). The use of datasets with higher frequency in space increase the complexity of simulation, however, significantly decrease the uncertainties.

Another important issues constitute the union of models which involved in SW-GW interaction. The union process involves several technical and technological aspects such as (i) coupling techniques, (ii) data integration (such as machine learning approaches), and (iii) output data. The framework of the combined models includes specified steps such as auto-generation of metadata, simulation verification, and automated recovery from system problems in the case of absence or limited input data (Badham et al., 2019).

Last but not least is the missing operator capabilities and fundamental knowledge. In many studies was obvious the high knowledge of hydraulic process and solving of mathematical problems, however the conceptual model was too weak due to the absence of the geological and hydrogeological background of the modeler. Contrariwise, application with detailed hydrogeological structure used limited simulation codes. To our opinion in the simulation process of GW-SW interaction should be involved a group of modelers with interdisciplinary background (engineers, geologists, environmentalists).

3 Discussion

The combination of GW-SW models provides an integrated simulation process, and a deeper understanding of Stream-GW interaction and spans a range of applications. The SW-GW interaction modeling process can provide essential information for the protection of both systems. Extreme hydrological events such as droughts and floods as well as human activities influence the SW and GW bodies. A lot of research has been applied worldwide for the investigation of various aspects such as the protection of water and cover of human needs (quality and quantity of water). Taking into consideration the general conclusions of the previous works, prevention is the most appropriate strategy in the fight against GW pollution/depletion (Patrikaki et al. 2012).

In total nine code combinations dominate in the case studies, while MODFLOW and SWAT constitute the most used models for the simulation of GW-Stream interaction worldwide. SWAT-MODFLOW model has been applied for the simulation of GW-SW interaction to contribute to agricultural problems, flood prevention and mainly for future projections of GW conditions. In most of the research cases, the authors applied SWAT-MODFLOW model for the evaluation of management aquifer recharge (MAR) practices. GSFLOW as the second most applied model contributes to agricultural problems, flood prevention and drought adaptation. HydroGeoSphere has been applied for the simulation of SW-GW interaction in the context of water resources management solutions concerning water scarcity and agricultural activity as well WetSpass-M–MODFLOW with an additional application in flood prevention scenarios. The comparison of HELP-FEFLOW and CATHY models has been applied for the conceptualization of aquifer and water exchanges between different configurations and combinations of boundary conditions. MODHMS and MIKE SHE-MIKE 11 models have been utilized for the conceptualization of water balance and contribution to agricultural problems for the suggestion of land use scenarios. FEFLOW-MIKE 11 models’ combination has been applied for future projection of climate conditions and impacts of surface runoff and GW recharge. HYDROLOG-AQUIFEM-N models have been utilized for the distribution of GW recharge rates from rainfall and water management practices.

The majority of GW-SW modeling approaches focused on GW reserves availability and future variability. The ever-increasing need for water along with the growing trend of the population, mainly in urban areas, and the increasing intensity of climate extreme events have led to the over-pumping of GW from year-to-year (Taylor et al., 2013). The study of GW depletion has been triggered by the overexploitation of GW in combination with the intense discussion of climate change. The increasing GW depletion is depicted by the results of forecasted simulation analysis worldwide (Dalin et al., 2017). The depletion of GW systems can be analyzed according to different scientific aspects (Aeschbach-Hertig and Gleeson, 2012). However, is important to follow a multidisciplinary approach in order to understand the phenomenon. It is essential to the conceptualization of both GW and SW systems. In the modeling process the hydraulic parameters of the aquifer and streambed are critical important for the simulation process. The importance of streambed and aquifer properties on the exchanging flux have been also highlighted by Tripathi et al. (2021). The measurements of hydraulic conductivity and hydrological fluxes between the river and the underlying aquifer are difficult due to their spatial and temporal transience. Tang et al., (2017) used geostatistical models (homogenous, Gaussian, non-Gaussian) of riverbed hydraulic conductivity within HydroGeoSphere model in order to increase the accuracy of exchange fluxes. The analysis of the hydraulic properties of streambed constitutes a crucial approach due to its properties are not constant (Gianni et al., 2016). The representation of the system's complexity is necessary to understand how natural and human systems function and interact. Sedimentation and erosion width of stream channels usually vary along the river due to physical (such as elevation, geology, plants, and animals) and anthropogenic factors (such as dam construction). The sediment transport process in river flow can be represented as a quasi-steady process. Although, it switches to suspended load, bed load, or mixed load depending on a transport mode parameter consisting of local flow hydraulics (Alexandrov et al., 2009). The characteristics of the vadose zone between riverbed and groundwater is also critically important due to the influence in both hydraulic and hydrochemical process (Schilling et al., 2017b). Higher thickness of the vadose zone decrease the fluxes form groundwater to river, while clay material in the vadose zone decrease the flux rates.

Another critical issue is the building of Dams which can significantly affect river systems. The flow modifications alter the flow and sediment in stream channels. Reduced flow also decreases tributary stream flow, changing habitats and altering the water table in the stream aquifer. It is essential to include the dam function in modeling of GW-SW interaction.

Due to the data availability is more feasible to build the conceptual model of surface hydro-systems. Contra-wise, GW system conceptualization constitutes a difficult procedure mainly due to the data scarcity (Khadim et al., 2020). Even in cases of abundance of data, researchers simplify the structure of the aquifer neglecting later changes in the lithology due to faults and preferential GW flow. Consequently, the section of the simulation code cannot provide accurate simulation results. A second issue for optimal and reliable simulation process is the extend and time step of time series inputs for the models. Obviously, the model demands are strongly connected with the nature of the problem. According to the literature overview, a daily step for a three-year period for both GW-Stream components constitute an optimal case for the modeling process. For future projections, the main input constitutes precipitation obtained from climate models and usually the time series is for a period of twenty years (Busico et al., 2021). Inevitably, during the simulation process many assumptions might be adopted mainly due to the lack of data. Nevertheless, many validation methods are available in the literature to accept the model. Haque et al. (2021) suggested strategies in detailed domain models highlighting the uncertainty in the simulation process due to the boundary conditions. The conclusions of this article are in accordance with the findings of this overview.

After the conceptualization of the hydrosystem and the validation of the simulation the model can be used under different scenarios.

In many of the applications, authors examined the optimal irrigation method to decrease the use of water. Some of the methods incorporated within the modeling process were: a) stream diversion for flood and sprinkler irrigation, b) irrigation supplied solely by GW, c) optimal water-use irrigation conditions that minimize the evapotranspiration (ET) deficit, and d) irrigation that is triggered when the ET deficit drops below a specified threshold. In some case studies, the modeling scenario involved land use and crop type changes. The concept incorporates the establishment of crops with low irrigation, fertilizers and pesticide demands in GW polluted and depleted zones.

The application of Managed Aquifer Recharge (MAR) constitutes another approach in the fight against GW pollution and depletion (Dillon et al., 2019). Managed Aquifer Recharge (MAR) has begun to be applied in the whole world to enhance and secure GW under stress (Sprenger et al., 2017; Dillon et al., 2018; Zhang et al., 2020). The application of these methods is considered necessary in areas where the natural recharge of aquifer is not feasible, or the infiltration recovery is slow and incomplete. MAR application can incorporate SW, treated wastewater as well as desalinated water. MAR is a complex and high-cost option, and GW simulation models should evaluate it fully before its large scale in situ application (Pliakas et al., 2005). Initially, Niswonger et al. (2017) studied the application of MAR by simulating SW-GW interaction.

Tran et al. (2020) used the physical-based numerical model GSFLOW to quantify the spatial and seasonal variations of water cycles affected by fluvial landform conditions and human activities. The modeling process contributed to the optimization of MAR application. Additionally, Salem et al. (2020) evaluated the feasibility of the natural reservoir based on water resources of the floodplain through SW storage. The authors applied Wetspass-M and MODFLOW NWT model and tried to analyse the restoration of natural reservoirs (abandoned paleochannels) and MAR technique to mitigate water shortage problems caused by drought and human activities. MAR can be also incorporated into DSSs which include numerical models to explore hypotheses and develop the optimum management activities (Lindhe et al., 2020).

In the last decades, new codes and software have been developed and are available to simulate complex hydrological phenomena. For instance, the modeling of GW-SW interaction can provide solutions to practical problems in agriculture, application of MAR and forecasting of water reserves. The increasing trend in modeling application is also triggered by the open access to worldwide data sets. Nonetheless, there are many future challenges and research needs to improve the accuracy in the modeling of GW-SW interaction.

3.1 Future challenges and research needs

The literature overview reviled that integrated modeling incorporating both SW components and GW is chosen by researchers to solve modern hydrogeological problems. Considering the ongoing studies, the following aspects can improve the modeling process of GW-Stream interaction:

- **Field monitoring**

  The calibration-validation process of SW-GW modeling requires in situ measurements of hydrological parameters. However, data are not always available to researchers. The data scarcity constitutes a deterioration factor for SW-GW interaction modeling. In many studies modeling is partly based on remote sensing and satellite data. Undeniably, the reliability of the modeling process is strongly linked to field data. In a hydrological basin, scale is essential to establish a station for high-frequency monitoring of surface runoff and quality, meteorological parameters and GW table level and quality. The station's number and locations are dependent on the extent of the site, the climatological characteristics and different aquifer types. The importance and cost of station maintenance and data collection must be considered, as the benefits that data availability can offer to SW and GW management are significant.

- **Tools to elaborate large data sets**

  The modeling process require large data sets with frequent acquisition of parameters. Within this study, the existence of several open access data bases that authors can retrieve is highlighted. Nevertheless, due to the extent of data series, the coding process is necessary to analyze and prepare the data to input into the different simulation software now available. Often, there are gaps in the data sets or incorrect measurements. Consequently, is necessary to fulfill the gaps and eliminate the biased data. However, easily applicable tools to overcome this issue are missing from the literature. It is essential to develop such tools to support the elaboration of a long period with frequent time-step hydrological data sets which are compatible with the available GW-SW simulation software.

- **Multidisciplinary analysis**

  The simulation of Stream-GW interaction incorporates several factors and processes. Several hydrogeological, geochemical, biological, and climatological aspects are involved. Many studies observed one-dimension analysis of data and/or absence of multi-factor interaction. Obviously, such analysis might explain individual processes, however, weakens the understanding of hydrosystem function. In future studies, the engagement of different disciplines should be involved in the simulation of Stream-GW interaction incorporating also biological and socioeconomic aspects. Furthermore, the combination of techniques with numerical flow models is an ever-growing area of research (Schilling et al., 2017). Decision Support Systems can contribute to multidisciplinary approaches incorporating modeling in the decision process to obtain integrated water resource management (Fredericks et al., 1998).

- **Riverbed variations**

  The modeling result is strongly dependent from the initial conceptual model of both groundwater and surface water systems. Groundwater systems have stable structures, however human intervention change groundwater flow and quality. Riverbed structure is variable from both natural phenomenon and human activities. Obviously, the variability of the conceptual model of SW-GW interaction is challenging for the simulation process (Brunner et al., 2017). Riverbed variations due to lateral mobility and vertical scouring can influence the hydraulic parameters of streambed and wetted depth and consequently the fluxes between surface water and groundwater. The variations of riverbed are not considered in SW-GW interaction modeling and researchers use constant parameters in space and time. The impact of such variations in GW-SW interaction is essential and strongly recommended to researchers in future studies.

- **Modeling limitations**

  Models constitute simplifications of nature and obviously are limited by underlying simplifying approximations (Anderson et al., 2015). Hence, different combinations of the inputs can produce data similar to field-measured ones. No uniqueness in modeling process is widely accepted and hence the right answer lies within the uncertainty limits (Doherty, 2011). The uncertainty of a model arises from several factors including heterogeneity of subsurface, unanticipated future stresses as well as the assumptions of the selected code. The uncertainty of a model cannot be eliminated; however, the model should be updated when new data are available. The uncertainty of the model can be decreased by using higher amount of data and accounting more process in the simulation. The high amount of data depict the complexity of hydrological systems (Fatichi et al., 2016; Schilling et al., 2019; De Filippis et al., 2020).

The limitations have been established by numerous authors, however, in the applications analyzed in the overview less studies are provided on the limitations of the model. Highlighting the limitations and uncertainty limits is fundamental in the presentation of modeling SW-GW interaction.

- **Ethics of modeling**

  The accuracy of the modeling results is not only dependent on the data availability, software capabilities and modeler skills. The modeler should plan, design, and simulate the process acting in a morally responsible manner. Thus, can be achieved when an accurate question is addressed, and the modeler build the model without approximations that bias the outcomes. Another factor that the modeler should address is the cost of the model process. Usually, the cost constitutes the main limitation factor to build an accurate model. The cost includes both data gathering and time to obtain the simulation. The presentation of the results is also a significant ethical factor. Brief presentation usually occurs when the uncertainty is high due to the lack of data, time to fulfill the simulation and in some cases when the modeling aims to underestimate the impacts of human activities on water resources. The importance of modeling ethics should not be neglected when an article is published. Nowadays numerous publications include models of GW, SW, and combined ones with a high range of uncertainty which are usually not presented. Additionally, in many case studies fundamental mistakes are obvious in the outcome. The increased water demands, water pollution and competitiveness between authors might be the reason for the model applications.

Within this study is not possible to provide all aspects of modeling GW-SW interaction. Nevertheless, the obtained literature overview of the existing case studies can trigger researchers to use the modeling technique to conceptualize a GW-Stream system, understand the interconnected process, solve complex hydrogeological problems, and contribute to solutions for integrated and sustainable water resource management. The establishment of monitoring stations with the consideration of the correct surveillance, the implementation, and the effectiveness can cover data gaps. Finally, we strongly believe that the establishment of legislative frameworks for high-frequency monitoring of GW and SW changes by municipalities and other relevant bodies is of utmost importance.

4 Conclusions

The interaction between SW and GW is a multifactor and interconnected process. Numerical modeling constitutes a reliable approach to understand such complex process and provide reliable answers to state-of-the-art problems. The detailed analysis of the obtained literature overview of GW-SW interconnection resulted in the following conclusions:

- There is an increasing trend to model water resources in an integrated manner incorporating both Stream and GW.
- New software and update codes simplify the simulation of GW-Stream interaction.
- MODFLOW-SWAT constitute the dominant approach within the existing literature.
- Data scarcity and lack of high frequency field measurements are the main limitation aspects of modeling process.
- Multidisciplinary approaches are essential to understand Stream-GW interaction.
- The modeling ethics should not be neglected during the modeling procedure.

The modeling of GW-Stream interaction is an ongoing process with uncertainties and unknown aspects. Is essential to undergo rigorous reconsideration of the model and adopt to new data findings. A next step of this study is an overview of solute transport and heat and density dependent transport. These processes are challenging considering the modern environmental issues on a global scale.

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Graphical Abstract

Highlights

a) An overview of simulations on GW-SW interaction worldwide was obtained.

b) SWAT-MODFLOW is the most used model for GW-SW modeling.

c) Data availability constitutes the main challenge for future application.

d) Simulation process is essential to mitigate GW depletion phenomena.