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Coupling of unsaturated and saturated flow modelling - a strong point of the small research catchment Uhlířská

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Coupling of unsaturated and saturated flow modelling

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Key Words

Numerical modelling, vadose zone, saturated flow, environmental isotopes, dual porosity, catchment water balance

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Novelty and International Appeal Statement

This manuscript presents a creative combination of numerical modelling approaches with computation of water balance and isotope-supported calibration to address a wide set of hydrological processes in the vadose and saturated zones of a headwater catchment. The methodology makes use of a nearly 30-year monitoring of diverse components in the research catchment Uhlířská, thus providing a contribution to this HP Special Issue on hydrological research catchments.

Data Availability Statement

Due to multiple funding constraints/subjects and third party data agreements use (CHMU, Povodi Labe, VUV, IAEA), no data for this study are publicly available. The authors however welcome cooperation and data sharing based on equality approach or welcome to share certain data pieces within initiatives where they decide to join based on their free decision. A citation of the isotope data retrieved from the IAEA databases are included in the References section of the manuscript.

Text File

Abstract

Modeling results in the small (1.78 km^2) experimental catchment Uhlířská located in the northern part of the Czech Republic at the average elevation of 822 m a.s.l. are presented. While the basic hydrological and meteorological monitoring has started already in 1982, investigation of the subsurface flow adjoined in 1995. A detailed survey of water and isotope (^{18}O, ^{2}H, ^{3}H, $^{3}H/^{3}He$) fluxes across the catchment storage compartments has been in operation since 2006. The combined vadose/saturated zones modeling with support of partial extrapolation of ^{18}O content in precipitation yielded the following mean balance for the period 1961-2014: 456 out of 1220 mm annual precipitation depth are percolating through the soil matrix domain and 534 mm through the preferential domain in the hillslope soil profile. The saturated zone is recharged annually by 416 mm, consisting of the entire matrix flow and 12,5 % of the preferential flow from the permeable hillslopes covered by Cambisols and Podzols, as well as by the contribution of 22 mm from the less permeable riparian wetland Histosols. The aquifer geometry was determined by means of electrical resistivity tomography (ERT) including inverse modelling (RES2DINV). Water and isotope fluxes were computed using a sequence of models. They include S1D software for the vadose zone modeling including ^{18}O transport and Modflow, Modpath and MT3DS determining residence time and flow trajectories in the saturated zone. Isotopes ^{3}H and $^{3}H/^{3}He$ improved the model confidence. The water residence time on the hillslopes does not exceed 1 year, while the saturated zone indicates about 10 years, with a 20% portion of water older than 100 years in the deepest part of the aquifer. The combination of numerical modelling approaches with computation of water balance and isotope-supported calibration is considered innovative, particularly the $^{3}H/^{3}He$ method to determine water residence times of young groundwater in the saturated zone.

1. Introduction

The coupling of vadose and saturated flow modelling has been more intensively addressed since the 1980's and 1990's upon the establishment of the software packages such as MODFLOW (McDonald & Harbaugh, 1984) for the saturated zone and FEFLOW (Diersch, 1981) for the unsaturated zone. These approaches were further developed in a variety of modified or newly developed codes (Harter & Morel-Seytoux, 2013; Chen, Ahmad & Kalra, 2018) or linkages between the saturated and vadose zones (Yi & Sophocleous, 2011; Facchi, Ortuani, Maggi & Gandolfi, 2004) or between streamwater and groundwater (Markstrom, Niswonger, Regan, Prudic & Barlow, 2008). Several authors have developed new integrated models (Kollet & Maxwell, 2006; Jones, Sudicky & McLaren, 2008; Camporese, Paniconi, Putti & Orlandini, 2010) instead of individual approaches for the respective catchment compartments. Very recently, Bizhanimanzar, Leconte, & Nuth (2020) used a groundwater flow model in a surface runoff simulation, concluding that a well parameterized groundwater model may require less input data than a surface runoff model, in addition to a higher computation efficiency especially at regional scale.

The coupling of model components of the unsaturated and saturated flow at the catchment scale typically includes uncertainties in the assessment of the boundary conditions between the individual catchment compartments (Barthel, 2006). In particular, it is very important to find a common definition and scale-appropriate process description in order to achieve a meaningful representation of the processes that link the unsaturated and saturated zones and the river network. In this context, several authors address boundary condition processes such as excess saturation and infiltration (Kollet & Maxwell, 2006), as well as aquifer replenishment (Welch & Allen, 2012) and geometry (Condon et al., 2020).

Since decades, the saturated and unsaturated flow model approaches have been linked to transport of tracers, in particular environmental isotopes. Whereas a substantial number of studies in the vadose zone (review in Barbecot, Guillon, Pilli, Larocque & Gibert-Brunet, 2018) addressed the use of isotopes in quantifying groundwater recharge, the dominant use in the saturated zone (review in Turnadge & Smerdon, 2014) has been focused on calibration of aquifer hydrodynamic parameters and estimation of groundwater residence times. In turn, little attention has been paid to the coupling of surface, subsurface and groundwater flow and transport modelling to quantify the fluxes and estimate the water balances in the individual catchment compartments and across their boundaries at different scales. In their very recent overall review, Blöschl et al. (2019) address this question as one of the twenty-one unsolved problems in hydrology.

Small research catchments have been traditionally used to elucidate concepts of water flow, storage, and residence, and generate hydrological datasets to calibrate and verify models (McDonnell, 2003). In the recent past, environmental tracers essentially contributed to the conceptual understanding of the subsurface and groundwater flow controls in numerous research catchments across the world (recent review in Hale & McDonnell, 2016; Hale et al., 2016). The small (1.78 km^2) experimental research catchment Uhlířská located in the northern part of the Czech Republic at the average elevation of about 822 m a.s.l. (exactly 776-886) has been part of the national and international hydrological research in research catchments since 1982, with a substantial expansion of research program and activities since 2007. The recent research in the humid temperate mountainous Uhlířská catchment revealed the dominant role of hillslope infiltration and preferential flow (Hrnčíř, Šanda, Kulasová & Císlerová, 2010; Dušek, Vogel, Dohnal & Gerke, 2012; Šanda, Vitvar, Kulasová, Jankovec, & Císlerová, 2013; Dušek & Vogel, 2018, Dušek & Vogel, 2019) as well as snowmelt (Šanda et al., 2017; Šanda**,** Vitvar, & Jankovec, 2019) in the runoff generation, and the role of riparian wetlands as main dissolved sulphate reservoir from acid rain inputs (Marx et al., 2017). Transport of oxygen isotopes through the vadose hillslope zone was modelled (Dušek, Vogel, Dohnal & Gerke, 2012; Dušek, Vogel, & Šanda, 2012; Dušek & Vogel, 2019) by use of the S1D software (Vogel, Gerke, Zhang, R., & van Genuchten, 2000), groundwater residence times were estimated using the $^3He/^3H$ approach (Jankovec, Vitvar, Šanda, Matsumoto, & Han, 2017) and the evolution of major ionic concentrations along subsurface water flow paths was assessed by the NETPATH approach (Vitvar et al., 2016). The conceptual knowledge of the dominant fluxes and interactions of the catchment compartments allowed to quantify the catchment water balance which is presented in this paper for the period 1961-2014. It is largely based on the recent thesis of Jankovec (2019) and combines available software packages into a unique innovative synthesis of modelling the unsaturated and saturated fluxes. We believe that this approach not only complements and summarizes the knowledge of hydrological processes in the Uhlířská catchment, but that it is also transferable to other catchments and can contribute to their intercomparison and classification.

2. Site description

The Uhlířská catchment (Fig. 1) is located in the Jizera Mountains near the northern border of the Czech Republic (50.8242289N, 15.1470839E). It is a small (1,78 km^2) forested headwater catchment with average altitude 822 m a.s.l. in cold humid climate, characterized by mean annual precipitation amount of 1300 mm and mean annual temperature 4.7°C (Hrnčíř, Šanda, Kulasová & Císlerová, 2010; Jankovec, 2019). The geological properties of the site were determined by their evolution as a part of Krkonoše-Jizera Composite Massif, which forms the northern region of the Bohemian Massif. The parental Jizera granite is classified as a medium-grained, strongly porphyritic biotite granite. Mineral soil hillslopes cover 1.45 km^2 (82% of the catchment area) and their 0.6 - 0.9 m thick soil profile consists of highly permeable Dystric Cambisols, Podzols or Cryptopodzols (Nikodem, Pavlů, Kodešová, Borůvka, & Drábek, 2013). As the hydraulic conductivity exceeds common precipitation intensities, all of the annual precipitation on the hillslopes infiltrates the soil profile without causing any direct surface runoff. Wetlands (0.33 km^2-18 % of the catchment area) along the stream course are formed by Histosol soil types. They are up to 4 m deep, with permeability values substantially lower as compared to the soils on the hillslopes. Wetlands are located on a layer of deluvio-fluvial sediments deposited in the catchment valley with a various depth reaching up to 50 m.

The vegetation cover on major part of the area has been completely altered by massive deforestation. Throughout history the area was covered by beech forest, but this was replaced by spruce in the 18th century as result of the rapid development of the glass and building industry. Air pollution during the period 1970-1980 resulted in large-scale dieback (40 to 80 percent) of spruce (*Picea abies*) stands; however, recent studies (Romanowicz, Kulasová, Ředinová, & Blažková, 2012) indicate that the differences in the catchment response in the Jizera Mountains to external climatic factors outweigh the influence of land use apart from the low flows, where the changes in the response might be attributed to afforestation. Spruce forest was naturally replaced by bush grass vegetation (*Calamagrostis villosa*). Once the air pollution was reduced in the 1990s, forests were planted with primarily spruce monoculture and a minor component of isolated beech (*Fagus sylvatica*), larch (*Larix decidua*) and crane (*Sorbus aucuparia*) trees. The wet soils, mainly at the bottom of the valley, are typically covered by peat moss (*Sphagnum*) species.

Basic hydrological and meteorological monitoring at the Uhlířská catchment has been operated continuously since 1982. The catchment (Fig. 1) is operated as a small research catchment by the Czech Hydrometeorological Institute (CHMI), in collaboration with the Czech Technical University in Prague (CTU), Czech Academy of Sciences (CAS), Czech Geological Survey (CGS) and other research organizations. A substantial expansion of the monitoring facilities towards the flow dynamics and pathways was performed in 1995 and 2007 by the CTU, followed by a series of national and international publications on the runoff, recharge and subsurface flow mechanisms (e.g., Hrnčíř, Šanda, Kulasová & Císlerová, 2010; Dušek, Vogel, Dohnal & Gerke, 2012; Šanda, Vitvar, Kulasová, Jankovec, & Císlerová, 2013; Šanda et al., 2017; Marx et al., 2017; Votrubová, Dohnal, Vogel, Šanda, & Tesař, 2017; Dušek & Vogel, 2018; Dušek & Vogel, 2019; Šanda, Vitvar, & Jankovec, 2019). Innovative monitoring approaches were also tested in the Uhlířská catchment, such as automatic minidisk infiltrometers (Klípa, Sněhota, & Dohnal, 2015) and quantitative neutron imaging of the water and entrapped air redistribution in heterogeneous soil samples (Sněhota et al., 2015). Experiments in the neighboring areas to the Uhlířská catchment revealed the role of stemflow-induced infiltration for the generation of toxic aluminum hotspots in the soil (Nikodem et al., 2010). The individual monitoring activities and results of previous research will be discussed in more details later in this paper. Part of the monitoring expansion since 2007 has been devoted to regular isotope (^{18}O, ^{2}H, ^{3}H) and periodical hydrochemical tracers. The catchment is also part of the International Atomic Energy Agency (IAEA) global networks GNIP and GNIR (Vitvar, Aggarwal, & Herczeg, 2007), and the Euromediterranean Network of Experimental and Representative Basins GEOMON (Fottová, 1995).

3. Data and Methods

The coupling of unsaturated and saturated flow modelling in the Uhlířská catchment from point to catchment scale included a sequence of approaches and datasets (Fig. 2). The principal modelling period covers the years 1.1.1961-30.4.2014 and consists of two subperiods: modelling subperiod during the extensive monitoring program between 1.5.2007 and 30.4.2014, and extrapolation subperiod back to 1.1. 1961.

Precipitation was monitored since 1996 at the Uhlířská station along the western catchment divide ("Weather station" on the Fig. 1). A correlation with the nearby (2.1 km away) station Bedřichov was performed during the period of parallel monitoring at both stations Uhlířská and Bedřichov (1.6.1996 – 1.2.2015), which provided the extrapolation of precipitation data at Uhlířská between 1961 and 1996. In a similar way, meteorological data measured in parallel at Uhlířská and BED in the period 1.5.2006 – 30.4.2010 were correlated and extrapolated for Uhlířská from 1961 until 1996. The meteorological parameters were transformed to hourly (vegetation season 1.5.-31.10.) and daily interval (dormant season 1.11.-30.4.) and served for computation of evapotranspiration loss from the unsaturated zone, using the Penman-Monteith method (Dohnal & Vogel, 2011, in Jankovec, 2019). The hydrological runoff monitoring in the Uhlířská catchment (station UHL, Fig.1) has been in operation since 1982. Discharge data are currently collected at 10-min intervals.

A set of 14 suction cups (depth 30 and 60 cm) and 4 shallow groundwater piezometers (depth 2.6-5.2 m) is located (Fig. 1) along the experimental hillslope transect approximately in the middle part of the catchment. The hillslope has a length of 25 m, the depth of the unsaturated zone is 75 cm, and the surface slope is estimated to 14 % (Dušek & Vogel, 2018; Dušek & Vogel, 2019; Jankovec, 2019). Water percolated through the hillslope vadose zone is captured in a trench located squarely to the hillslope in the depth of 75 cm, which is considered the boundary of the vadose zone (Dušek & Vogel, 2018; Dušek & Vogel, 2019; Jankovec, 2019). The outflow water in the trench is monitored by use of a tipping bucket and sampled for ^{18}O and ^{2}H analyses. Since 2007, the sampling in the trench is performed in a 6-hour interval while event water is present and the sampling in the boreholes and suction cups is performed monthly. Snow depth is monitored on the experimental hillslope in the vicinity of the trench and snow samples are collected approximately in a weekly step. These facilities served for calibration of the transport of ^{18}O through the unsaturated zone during the calibration period 2007-2014.

The analyses of ^{18}O were carried out at the Czech Technical University in Prague, using the Liquid Water Isotope Analyzer, LGR Inc. device (Penna et al., 2010). The values are expressed as d^{18}O in ‰ of V-SMOW with typical precision of ±0.15 ‰ V-SMOW. Contents of ^{18}O in precipitation and at the streamflow catchment outlet (UHL) have been analyzed since 2007 in monthly samples within the framework of the IAEA isotope hydrology databases GNIP and GNIR (Vitvar, Aggarwal, Herczeg, 2007).

Three nearby 10-cm diameter wells (HV) were drilled in 2009 in the vicinity of the catchment runoff gauge UHL. The wells are denoted HV1C, HV2B and HV3A with depths of 10, 20, and 30 m screened at 8-9, 18-19 and 28-29 m depths, respectively. The wells are 5 m apart in a line and can therefore be considered as a single multi-level well. The uniform water table in all wells suggests a single aquifer over all three depths. Samples to describe grain-size distribution of the sedimentary aquifer near the catchment outlet were collected during the core drilling. Granulometric composition of the core samples indicates a homogeneous structure of the material along the boreholes (Jankovec, 2019). The absence of material with significantly different composition is in agreement with electric resistivity tomography (ERT) measurement results and supports the idea of a consistent sand-gravel layer of sediments in the valley part of the catchment. There wells were used to the calibration of the saturated model by the $^{3}He/^{3}H$ method. This isotope in combination with its daughter product ^{3}He has been often used to determine the mean residence time of shallow groundwaters, because the usually muted seasonal variations of common stable isotopes ^{18}O and ^{2}H in groundwater do not allow for an undoubtful interpretation of residence times. (Schlosser, Stute, Dorr, Sonntag, & Munnich, 1988). The groundwater samples for this isotope analysis were collected in three campaigns (May 2011, October-November 2011, May 2012). They were processed and analyzed in the IAEA's Isotope Hydrology Laboratory in Vienna by using a sector field noble gas mass spectrometer (Micromass 5400) for helium isotopes and quadroupole mass spectrometers for neon, argon, krypton and xenon isotopes (Suckow, Gröning, Jaklitsch, Han, & Aggarwal, 2008). Water samples for tritium analysis were subjected to distillation, electrolytic enrichment and the low-level decay counting by liquid scintillation counting (Quantulus 1220™) in the IAEA's Isotope Hydrology Laboratory with a detection limit of about 0.4 TU (Wassenaar, Kumar, Douence, Belachew, & Aggarwal, 2016).

Geophysical measurements by means of multicable electrical resistivity tomography (ERT) (Beauvais, Ritz, Parisot, Bantsimba, & Dukhan, 2004) were performed across the whole catchment in 7 profiles, of which 6 is transversal to the main stream axis (A-F) and cross ing the hillslopes and valley and one is longitudinal – parallel to the stream valley (T) (Fig. 1). ARES G4 device (GF Instruments, s.r.o.) with distant controlled electrodes has been used in 5 m spacing with total of 40 pieces, i.e., 195 m long profile section (A-F) and 56 pieces, i.e. 275 m profile section (T) has been measured at a time, leaping 24 (A-F) and 30 (T) electrodes to the next section, thus creating overlaps. Vertical reach was approximately 40 m (A-F) and 55 m (T). Apparent resistivity has been reconstructed using RES2DINV inversion modelling (Loke, 2001).

The sequence of the components for the integrate flow and transport modelling (Fig. 2) included four principal packages: the S1D (Vogel, Gerke, Zhang, R., & van Genuchten, 2000) to simulate the flow and transport in the vadose zone, the MODFLOW, MT3DMS (Zheng, 2010) and MODPATH (Pollock, 2012) to simulate the flow and transport in the saturated zone, the BFLOW (Arnold, Allen, Muttiah & Bernhardt, 1995) for estimation of overall baseflow contribution to streamflow (and, therefore, to validate the modelled overall input to the saturated zone) and the closed-system equilibration (CE) model to estimate groundwater residence times by use of the $^{3}H/^{3}He$ approach (Aeschbach-Hertig, Peeters, Beyerle, & Kipfer, 2000; Schlosser, Stute, Dorr, Sonntag, & Munnich, 1988).

The unsaturated flow and transport were simulated by use of the S1D approach (Vogel, Gerke, Zhang, R., & van Genuchten, 2000; Vogel, Březina, Dohnal, & Dušek, J., 2010) in two domains: the soil matrix and the preferential flow macropores. The unsaturated flow according to Richards equation is considered vertical in the soil matrix until the bottom boundary of the unsaturated zone is reached. In turn, the lateral preferential macropore flow is conceptualized parallel to the hillslope. The application of this approach in the Uhlířská catchment consisted of two separate steps: a) modelling the instrumented experimental hillslope (Fig. 1, 82 % of the catchment area) with a subsurface slope of 14 % and length of 25 m, and b) modelling the riparian wetland along the stream course (18 % of the catchment area). Based on previous geophysical surveys, the hillslope was conceptualized by both domains (soil matrix and preferential pathways), whereas the wetland was conceptualized by matrix domain only. The modelling was performed in two intervals – calibration in short term (seasonal – summer and winter) intervals between 2007 and 2014, and long term extrapolation for the whole period since 1961. The summer periods were calibrated in hourly intervals, whereas the winter periods were calibrated in daily intervals. The input to the unsaturated model was precipitation subtracted by evapotranspiration, and the output from the unsaturated zone included both the trench flow, attributed to the rapid macropore domain, and the recharge to the saturated zone, attributed to the soil matrix domain. Hydrodynamic parameters (porosity, permeability) and the portions of both the soil matrix and macropore domains were iteratively calibrated for each summer and winter period, and then applied in the extrapolation of the unsaturated flow for the period back to 1961 (Jankovec, 2019).

The maximal depth of the saturated zone of 55 m was determined using the previous geoelectrical survey (Jankovec, 2019). The aquifer was divided into 7 depth zones of 5 to 10 m depth. The modelling of the saturated zone was carried out in monthly step using the flow (MODFLOW2000) and transport (MT3DMS) modules (Zheng, 2010) and the particle tracking package MODPATH (Pollock, 2012). The graphical interface and data processing were performed using the Groundwater Vistas package (Rumbaugh & Rumbaugh, 2015). Shallow piezometers and deep boreholes were used for the calibration of the saturated zone flow between each of the 7 layers. The remaining groundwater flow was then attributed to the groundwater subsidy to the lower catchment.

To verify the modelled estimation of the recharge to the saturated zone, the long term baseflow contribution (baseflow index, BFI) to the total streamflow at the Uhlířská stream gauge was estimated by means of the BFLOW package (Arnold, Allen, Muttiah & Bernhardt, 1995) for daily discharges between 1.1.1982 and 30.4.2014. This approach analyzes the frequency spectrum of daily hydrographs, associating long waves with baseflow and high frequency variability with direct runoff. The baseflow index was determined through three-step filtering of hydrograph with daily flow values and expressed in % as the baseflow portion of the total streamflow. The long term average baseflow amount was used as independent verification value to the simulated input to the upper model layer of the saturated zone. It was hypothesized that both these values (average input to the saturated zone and average baseflow in the stream) would result very close to each other.

4. Results and discussion

The initial input to the model sequence of the vadose and saturated zones at Uhlířská included the precipitation and evapotranspiration data. Based on the parallel monitoring period at the stations Uhlířská and Bedřichov (1.6.1996 – 1.2.2015), extrapolated precipitation values for the station Uhlířská in the period 1.1.1961-31.5.1996 were determined. The average annual precipitation amount for the entire period 1961-2014 is 1220 mm. This is approximately twice as high as the average annual precipitation in the Czech Republic (672 mm according to the Czech Hydrometeorological Institute, for the period 1961-2018). This confirms the overall humid climate of the study zone. The mean annual evapotranspiration rate of 230 mm was computed, which also corresponds to the common values in the temperate humid Central European mountains.

Modelling of the vadose zone

The application of the S1D model for the unsaturated flow was based on the previous field and modelling studies summarized in Dušek, Vogel, Dohnal & Gerke (2012), Dušek, Vogel, & Šanda, (2012), Dušek & Vogel (2018) and Dušek & Vogel (2019). They resulted in an experimental (from soil samples) determination of the matrix (95 %) and macropores (5 %) domains in the unsaturated layer along the hillslope profile at Uhlířská. The calibration for the period 2007-2014 addressed the soil water presence (capillary retention – volumetric water content and hydraulic conductivity parameters in 7 vegetation seasons and 7 dormant seasons, each of which was separately calibrated against the trench outflow in the 75 cm depth below the terrain. The adopted modelling concept assumed rapid vertical percolation through the macropore domain (95 %) toward the trench, which later converted to lateral interflow towards the stream, and slower water movement through the matrix domain (5 %), attributed to groundwater recharge. The day-degree method was employed to convert snow cover into snowmelt input to the unsaturated zone (Jankovec, 2019). The modelling and calibration were performed in hourly step (vegetation seasons) or daily step (dormant seasons), respectively. The initial unsaturated hydraulic conductivities were also adjusted according to the infiltration experiments (Klípa, Sněhota, & Dohnal, 2015). The macropore runoff responses in the trench were rapid and of episodic character. Jankovec (2019) stated that the entire period 1961-2014 (calibration 2007-2014 and extrapolation 1961-2006) included 641 response events through the macropore domain. Jankovec (2019) also examined the role of the rooting depth in the model calibration, stating that the variation in rooting depth (and, therefore, potential changes in the evapotranspiration loss) caused little impact on the calibration process.

The unsaturated flow modelling was further coupled with ^{18}O transport module which is included in the S1D package. The ^{18}O precipitation input was determined from continuous electronically driven incremental ^{18}O monitoring of liquid precipitation at the Uhlířská station since May 2006. A sample includes either one day with 1-10 mm of precipitation, or each 10 mm of precipitation within any time interval. The period of 10 years of this ^{18}O monitoring in precipitation (May 2006 – April 2016) was correlated with the air temperature to determine the ^{18}O content in precipitation extrapolated back until 1961. The S1D transport module was then calibrated against the monthly measured ^{18}O values in the suction cups in depths of 30 and 60 cm and in the outflow trench. Fig. 3 shows the comparison of the simulated ^{18}O contents with the monthly measured ^{18}O contents in the suction cups. Higher annual maximum ^{18}O values in the depth of 30 cm are observed in comparison to the depth of 60 cm. This is probably attributed to the isotopic enrichment by evapotranspiration in the upper soil layers (Jankovec, 2019). The results of the combined flow and transport through the hillslope yield a mean annual balance of 456 mm in the matrix and 534 mm in the preferential domain (Fig. 4). Whereas the hillslope preferential flow is dominantly supplying the wetland and the stream (as conceptualized by silica tracers in Šanda, Vitvar, Kulasová, Jankovec, & Císlerová, 2013), the matrix flow was entirely attributed to groundwater recharge.

A separate simulation of flow and transport was carried out in the low permeable wetland located along the stream course on a Histosol soil type. Ponded infiltration measurements for the wetland area resulted in values of around 5 cm.d^{-1}, compared to 5000 cm.d^{-1} for the hillslope preferential domain and 17-67 cm.d^{-1} for the hillslope preferential domain (Šanda, Novák, & Císlerová, 2007; Klípa, Sněhota, & Dohnal, 2015; Dušek & Vogel, 2019; Jankovec, 2019). Studies of ^{18}O and silica in the catchment show that the wetland is largely supplied by groundwater or lateral preferential flow and, due to low permeability, transmits water to the stream by old artificial drainage structures (Šanda, Vitvar, Kulasová, Jankovec, & Císlerová, 2013). This wetland was therefore conceptualized as an unsaturated matrix with vertical percolation and modelled solely by the matrix domain of the S1D package. The S1D simulation of the percolation through the wetland was also calibrated against ^{18}O concentrations in the suction cups. Because the water in the higher permeable deluvio-fluvial sediments below the wetland layer shows ascending hydraulic communication with the wetland water (Šanda, Vitvar, & Jankovec, 2019), the seasonal fluxes between the wetland and the sediments may be of ascending or descending direction. The net mean annual recharge of 22 mm was computed from the wetland downwards to the sedimentary aquifer. (Fig.4).

Modelling of the saturated zone

The modelling of the saturated zone was supported by electromagnetic resistivity tomography (ETR) that identified saturated bodies of groundwater as well as solid, fissured and weathered granite (Fig. 5). The approximate maximum depth of the catchment aquifer of about 55 m was determined and the volume of the aquifer was estimated to $10E^7$ m^3. The maximum depth of 55 m was divided in seven model layers of variable thickness, with the most upper and two most lower layers of 5 m and the remaining four layers of approximately 10 m. This model structure supports the model calibration, because the screens of the deep (10, 20 and 30 m) boreholes near the catchment outlet will be situated in the middle of the 2nd, 3rd and 4th model layer. The input to the uppermost layer of the saturated zone was provided by the S1D- computation of the outflow from the unsaturated zone. The matrix flows through both hillslope (456 mm) and wetland (22 mm) were fully attributed to groundwater recharge, whereas the dominant portion (469 mm) of the preferential flow was attributed to lateral outflow. This corresponds to the previous conceptual findings in the catchment (Hrnčíř, Šanda, Kulasová & Císlerová, 2010; Šanda, Vitvar, Kulasová, Jankovec, & Císlerová, 2013). However, the calibration of the saturated zone modelling showed that using the recharge quantities from the matrix only led to a discrepancy between the computed groundwater discharge and the stream baseflow. To address this problem, Šanda**,** Vitvar, & Jankovec (2019) have used ^{18}O to assess seasonal variations in groundwater recharge in the Uhlířská catchment. They have identified depleted ^{18}O concentrations in spring and summer baseflow, which revealed that groundwater during snowmelt was recharged not only by the soil matrix, but also by a portion of the preferential domain flow. A recalibration of the model (Jankovec, 2019) showed that in average 12 % (65 mm) of the preferential domain flow contribute to the groundwater recharge. Hence the mean annual input to the saturated model from the hillslope consisted not only of the soil matrix flow (456 mm; matrix occupies 95 % of the total hillslope soil volume), but also of a 12 %-contribution of the preferential domain flow (65 mm; preferential domain occupies 5 % of the total hillslope soil volume). The preferential domain contribution was dominantly attributed to snowmelt periods. The total mean annual input to the saturated zone from the hillslope was therefore 416 mm, combining the contributions from the matrix and from the preferential domain. This balance has proven to be largely consistent with the previous findings in the catchment and with the modelling concept (Fig. 4).

The stationary groundwater flow within the seven model layers was simulated in a 10 m-grid in monthly step by the MODLOW 2000 package and calibrated against the water table values in the valley piezometers drilled through the peat wetland and the deeper boreholes near the catchment outlet. The total number of model cells over the whole aquifer was 211 827. However, only 67 294 model cells were used in the numerical solution, because the area of the layers decreases with the depth (Jankovec, 2019). The distribution of the saturated layers was adjusted upon the results of the electrical resistivity studies. The water table depths in the valley bottom are of about 20 cm, whereas the water table toward the headwaters is about 50 cm deep. The initial values of saturated hydraulic conductivity, storativity and effective porosities were inserted into the model according to common literature and previous local granulometric experiments (Jankovec, 2019). Tab. 1 summarizes the fluxes through the sequence of layers, revealing the most abundant fluxes in the 1st model layer. These fluxes (Fig. 4) dominantly supply the stream baseflow via the bottom valley deluvio-fluvial sediments (Jankovec, Vitvar, Šanda, Matsumoto, & Han, 2017; Šanda, Vitvar, Kulasová, Jankovec, & Císlerová, 2013; Šanda**,** Vitvar, & Jankovec, 2019). The calibrated saturated hydraulic conductivities in the 1st model layer decrease from the valley (2.5×10^{-5} m.s^{-1}) to the upper hillslopes (2×10^{-7} m.s^{-1}) and the effective porosities decrease from the valley (8 %) to the hillslopes (1 %). Fig. 6 shows that the first model layer has the most heterogeneous distribution of saturated hydraulic conductivity values, which implies a heterogeneous distribution of recharge and discharge zones in the shallowest layers. The deeper layers have lower calibrated conductivities (1×10^{-7} m.s^{-1}) and more uniform flow trajectories. The groundwater flow paths are typically oriented from the hillslopes downwards to the stream; however, a small portion of 16mm of the groundwater flow has a parallel direction to the stream and leaves the Uhlířská via deep flow paths towards the lower adjacent catchment (Tab. 1). Comparison of the mean modelled recharge to the saturated zone (24.2 $l.s^{-1}$, see Fig. 4 and Tab. 1) with the mean stream baseflow of 23.6 $l.s^{-1}$ obtained by the BFLOW approach for 1982-2014 (Arnold, Allen, Muttiah & Bernhardt, 1995) shows a very good agreement. This provides a further rationale for the conjunctive use of independent hydrological and groundwater modelling approaches in the Uhlířská catchment.

The transient MT3DMS model was used to simulate the transport of the environmental isotope ^3H through the saturated zone to the wells HV1C, HV2B and HV3A. The ^3H content on precipitation in the Uhlířská catchment was measured monthly between 2007 and 2014. The values for the period between 1961 and 2006 were extrapolated by using the correlation with the IAEA dataset at the Vienna station (IAEA/WMO 2020). Jankovec (2019) indicated that the ^3H input to the saturated zone (starting point of the ^3H-^3He isotope "clock") was by approximately 15 % lower than the ^3H in precipitation, due to evapotranspiration losses of typically ^3H-enriched summer precipitation. The adjusted ^3H-input became object of decay to conservative ^3He in the saturated zone revealing groundwater residence time in the wells HV1C, HV2B and HV3A of about 5, 20 and 40 years, respectively (Jankovec, Vitvar, Šanda, Matsumoto, & Han, 2017). The evolution of ^3H contents in the three wells is depicted in Fig. 7 and shows a good agreement with the measured values in the wells. It has to be noted that the y-axis shows the concentrations of the ^3H decay product ^3He; therefore, the oldest water (30 m deep) has the highest ^3He content, due to the longest decay time of ^3H. The slight discrepancy between the measured and modelled ^3He contents at HV2B might be explained by a possible admixture of younger (^3He-depleted) water. It is evident that a longer record of $^3H/^3He$ results would improve the model calibration; however, this approach has shown that the $^3H/^3He$ approach is an efficient tool to support the transient transport modelling in the saturated zone. Using the groundwater residence times in the three wells of 5, 20 and 40 years, and assuming average effective porosities from 0.15 to 0.30, Jankovec, Vitvar, Šanda, Matsumoto, & Han (2017) have determined the mean percolation velocity in the saturated zone 0.6 $m.y^{-1}$ and a recharge to the deeper aquifer zone of about 90-180 mm (7-14 % of annual recharge). This is consistent with the Tab. 1 in this study: about 1/3 of the recharge (30 % of 416 mm) percolates from the upper model layer to the second and third layers where the wells HV1C, HV2B and HV3A are located (10, 20 and 30 m of depth).

The modelling of the saturated zone revealed not only a heterogeneity of saturated hydraulic conductivity values, but also of groundwater residence times and $^3H/^3He$ concentrations. It appears that the first, second and third layers, which receive most of the recharge, show (Fig. 6) higher saturated conductivities along the slopes on the Eastern side of the catchment in comparison to the Western side. This is in agreement with higher modelled (Fig. 8) residence times and $^3H/^3He$ concentrations (Fig. 9) in the Eastern layers (up to 40 years in the third layer), where higher infiltration rates and more efficient mixing are hypothesized. The 4th layer shows a rather uniform distribution of saturated hydraulic conductivity values, but lower residence times in the Eastern sector. This indicates that the low groundwater input to the fourth layer and other deeper layers (Tab. 1) may contain relatively younger waters percolated relatively rapidly via saturated preferential flow paths from the upper layers (see also the above discussed discrepancy between the simulated and measured $^3H/^3He$ contents in the well HV2B). These hypotheses remain to be addressed not only in the Uhlířská catchment, but in catchment hydrology in general. We agree with the recent review of Condon et al. (2020) which states that assessment of "*Depth to low conductivity boundary"* and *"Active circulation depth"* are the key lines in the modelling of the deeper groundwater fluxes in catchments; however, we believe that the crucial way forward cannot be fulfilled only by combinations of unsaturated and saturated flow modelling and geophysical survey, but must be combined with environmental tracers, both isotopic and hydrochemical.

5. Conclusions

The presented paper showed that the research catchment Uhlířská poses a thorough and diverse monitoring and modelling concept to address the contemporary research needs. The strongest evidence of this concept is the variety of field datasets (hydrometeorology, hydrology, "traditional" and "less traditional" isotopes, geophysics) that was used in a combination of approaches to address the whole spectrum of catchment processes in the vadose and saturated zones. Although the used numerical approaches are relatively known and readily used commercial/academic packages (such as S1D, MODFLOW 2000 and the processing and visualization aggregates), we believe that a combined application of these tools offers advantages in comparison to building individual catchment models that need often require substantial adaptation and transfer effort to other catchment settings. The previously (since the 2000s) elaborated and published concepts in the Uhlířská catchment were not only confirmed by the presented combined unsaturated-saturated numerical flow and transport modelling, but the modelling vice versa revealed open questions that a numerical modelling alone would not address properly.

The used model components certainly include several drawbacks that must be carefully addressed in every application case. Although the S1D package has proven a wide application spectrum and flexibility in the combination with the transport component, it remains limited to 1D, which may challenge the modelling of complex transition zones such as the hillslope-wetland relation in the Uhlířská catchment. The irregular distribution of calibration wells may cause difficulties in the saturated flow and transport modelling, which need to be solved by environmental tracers. It is of utmost importance to simulate transport of independent tracers in both vadose and saturated zones (for example, ^{18}O in the vadose and $^{3}He/^{3}H$ in the saturated) to address transport at different time scales. The tracers did not only serve for model calibration (such as the ^{18}O in the S1D), but also revealed possible discrepancies between the $^{3}He/^{3}H$ breakthrough curves and the $^{3}He/^{3}H$ measured values in the wells (HV2B). Although the basic model approaches for the saturated and vadose zones (MODFLOW 2000 and S1D) are fully independent between the two zones, we do not consider this as a significant weakness, because a good conceptual knowledge of the processes allows a rational transition of values between these packages. Several alternative (and perhaps more detailed) modelling and parameterization strategies may be employed across other research catchments worldwide, we think that the presented study is a reliable way in catchment research and practice alike.

The presented long term monitoring is a strong component of the Uhlířská research catchment. It has not only been diverse in terms of monitored parameters, but it also offers long local datasets with backup or complementary datasets from nearby sites. This allowed to perform a two-step water balance, with a calibration period 2007-2014 and an extrapolation period back to 1961. We believe that such a database can serve to a wide variety of new and innovative conceptual and modelling tools in the Uhlířská research catchment and other sites worldwide.

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