

Catchments as reactors: a comprehensive approach for water fluxes and solute turnover

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Received: 4 October 2012 / Accepted: 23 January 2013 / Published online: 16 February 2013
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Abstract Sustainable water quality management requires a profound understanding of water fluxes (precipitation, run-off, recharge, etc.) and solute turnover such as retention, reaction, transformation, etc. at the catchment or landscape scale. The Water and Earth System Science competence cluster (WESS, <http://www.wess.info/>) aims at a holistic analysis of the water cycle coupled to reactive solute transport, including soil–plant–atmosphere and groundwater–surface water interactions. To facilitate exploring the impact of land-use and climate changes on water cycling and water quality, special emphasis is placed on feedbacks between the atmosphere, the land surface, and the subsurface. A major challenge lies in bridging the scales in monitoring and modeling of surface/subsurface versus

atmospheric processes. The field work follows the approach of contrasting catchments, i.e. neighboring watersheds with different land use or similar watersheds with different climate. This paper introduces the featured catchments and explains methodologies of WESS by selected examples.

Keywords Water and solute fluxes · Water quality · Catchments · Land-surface atmosphere exchange · Processes and feedbacks · Modeling · Monitoring

Introduction

Sustainable water management poses a big challenge in many countries worldwide (United Nations 2012;

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Vörösmarty et al. 2000). Besides water availability, the quality of water becomes increasingly important especially if water scarcity is involved (USGS 2007; Zimmermann et al. 2008, Nature News 2008). Degraded water quality affects ecosystem health, and it may propagate through the food chain, finally impacting human health and as such also translating into large economic damages (World Economic Forum Water Initiative 2009). While relevant processes contributing to water quality occur on a wide range of scales in space and time, water management is mainly conducted on a nested scale approach reaching from catchments to river basins (EU-WFD 2000).

Recent advances of in situ and remote-sensing methods and the development of coupled numerical models allow monitoring and simulating water and solute fluxes across compartmental interfaces at the catchment scale. This makes it possible to explore scenarios of land-use and climate change (Bates et al. 2008) and the potential impact and cost-benefit of management options on water quality. The research initiative WESS (Water and Earth System Science Competence Cluster) founded by the Universities of Tübingen, Stuttgart and Hohenheim together with the Helmholtz Centre for Environmental Research—UFZ, participates in these developments via a systems approach. WESS combines new monitoring methods with computational advances in order to address water and solute fluxes at the catchment scale as a function of and in feedback with changes in climate, land use, and water usage (see Fig. 1 for illustration). Of particular relevance is the fate of pollutants that are introduced by diffuse or non-point sources

(atmospheric deposition, agricultural application, infiltration and emission from urban areas). The goal is to develop probabilistic quantitative projections of the water cycle and of water-resources quality at the catchment scale in a changing environment. This requires assessing the naturally and anthropogenically modified environmental inventory, sound understanding of processes and system behavior including feedback mechanisms (e.g. of the land surface–vegetation–atmosphere system), advancing techniques for up-, downscaling and reduction of model complexity, and developing models that include both natural feedback processes and the impacts of human activities and decisions.

The field work of WESS follows the concept of contrasting catchments. The featured catchments differ strongly in land use, input of solutes, geology, morphology and climate (see Table 1). Cost-efficient monitoring strategies and novel measurement techniques such as online sensors and passive-sampling networks are developed and applied. Natural and anthropogenic compounds as well as isotopes are utilized as tracers in order to elucidate the origin and transport pathways of pollutants. High spatial and temporal resolution of the data is required to validate process-based models of the catchments. Data sets will be made available to the scientific community by the use of online portals.

The data collected in these catchments are used to inform numerical models that describe water fluxes, subsurface structures, the input of pollutants and other trace compounds and their reactive behavior in the subsurface and in the atmosphere as a coupled system. These models,

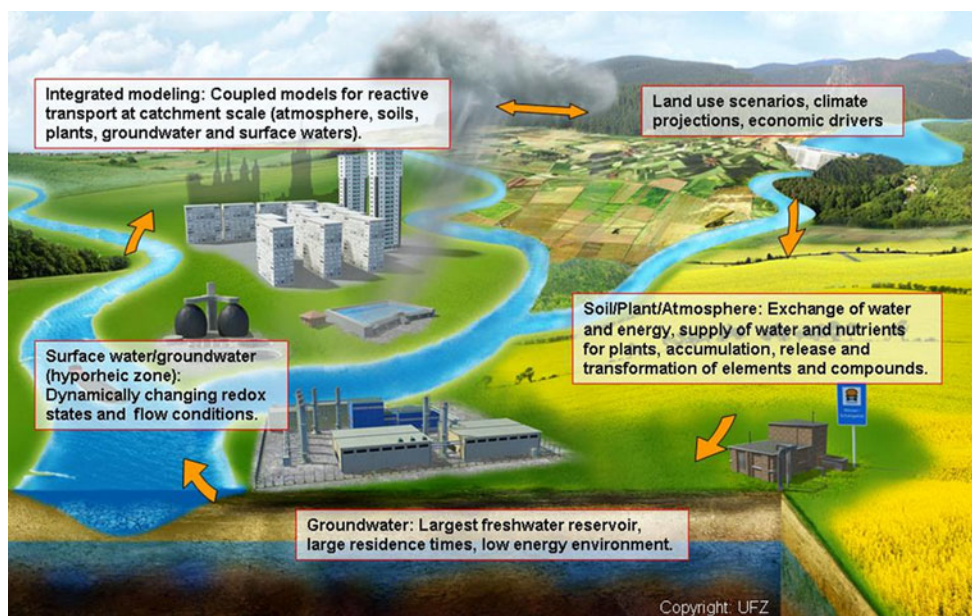


Fig. 1 WESS workflow from the soil–plant–atmosphere to the groundwater–surface water interface including integrated modeling and future climate and land use scenarios

Table 1 Most important characteristics of the WESS reference catchments in the upper Neckar and Bode areas

	Upper Neckar					Bode		
	Goldersbach	Steinlach	Ammer	Echaz	Körsch	Bode	Selke	Schäferthal
Gauging station	Bebenhausen	Tübingen	Pfäffingen	Wannweil	Mouth	Staßfurt	Hausneindorf	Schäferthal
Latitude	48°33'35'	48°29'26'	48°31'34'	48°31'22'	48°42'59'	51°51'17'	51°50'28'	51°39'16'
Longitude	9°02'34'	9°03'57'	8°57'51'	9°08'40'	9°21'32'	11°34'58'	11°15'55'	11°02'59'
A (km ²)	39	138	134	133	129	3,300	456	1.44
Land use								
Agriculture (%)	5	49	71	41	53	70	58	95 ⁽⁺⁾
Forestry (%)	93	39	12	35	13	22	35	3 ⁽⁺⁾
Urbanized (%)	2	12	17	24	34	8	7	
Main geologic feature	Sandstones, mudstones	Limestones, mudstones	Limestones, gypsum	Limestones, mudstones	Mudstones	Shales, sandstones	Shales, sandstones	Shales
Mean discharge (m ³ s ⁻¹)	0.25	1.75	0.96	2.8	1.4	13.0*	1.8*	0.0055
Mean specific discharge (l s ⁻¹ km ⁻²)	6.4	12.6	7.2	21.1	10.9	3.9	3.9	3.8
Mean runoff (mm yr ⁻¹)	202	397	226	664	342	124	124	120
Mean annual precipitation (mm) [#]	810	905	765	920	755	630	600	725

* HVZ, Sachsen-Anhalt (2012)

⁽⁺⁾ Ollesch (2008)

[#] 1980–2009; source: REGNIE data base, DWD

trained under current conditions, will be used to predict the impacts of changing environmental conditions and potential counteractive measures. Our approach starts with comparably complex, process-based models of the system at the catchment to river-basin scale that explicitly account for interactions between processes and compartments. Such models may be simplified to conceptual or surrogate models at a stage when the main interactions have been identified. Integrated numerical models are also a prerequisite for an economic evaluation of management strategies and technologies. The reliability of the simulations depends on the quality of the data fed into the models, the understanding of relevant processes, and the accuracy of the numerical codes. The large amount of data needs to be processed using innovative data assimilation techniques. Finally, massive parallel codes have to be developed that simulate reactive transport at the catchment scale over time periods of decades to centuries.

In general, sound model-based projections of future scenarios require:

- A profound understanding of the relevant (single) processes in different environmental compartments, mechanistic and process-oriented descriptions of these processes, and improved understanding of their mutual interactions in a coupled system.
- A coordinated approach of model building, experimental investigations and process monitoring at the field scale.
- The assessment of uncertainties, e.g. via probabilistic modeling approaches, for improved interpretation of modeling results, on which management decisions rely.
- Model validations at well-characterized reference catchments.

The objective of this paper is (i) to introduce the characteristics of the contrasting reference catchments that were chosen to test the interdisciplinary research strategy of WESS (ii) to provide an overview of new monitoring, modeling, and up-scaling concepts in order to identify and describe processes within the different environmental compartments and across compartmental interfaces (the land surface—atmosphere interface and the river—groundwater interface), and (iii) to provide concepts for integrated modeling of the complex catchment systems including innovative tools for model calibration, uncertainty estimation, and model-based optimization of monitoring strategies.

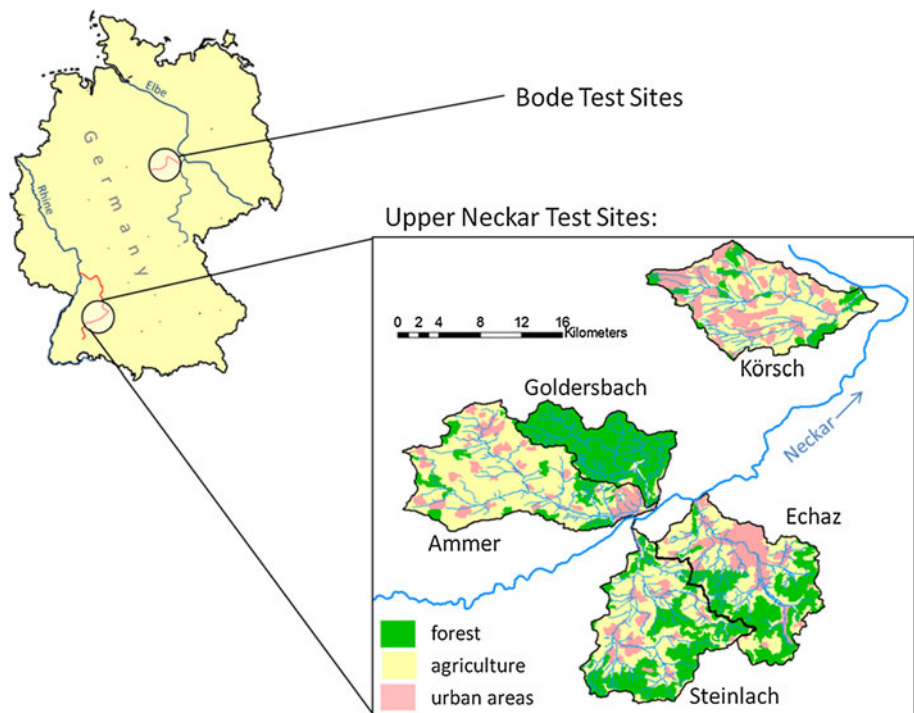
Contrasting catchments

For WESS, several reference catchments were chosen ranging in size from 1.4 to 3,300 km² (see Table 1 for main characteristics). The impact of different land use is

investigated in selected and contrasting reference catchments (Fig. 2) in the upper River Neckar Basin (tributaries Ammer, Goldersbach, Steinlach, Körsch). A nested monitoring and modeling approach is implemented in sub-catchments of River Bode in eastern Germany (Bode > Selke > Schäfertal). With this approach we build up on earlier catchment scale studies addressing, e.g., forest decline or acidification of soils and extend that to a more comprehensive range of water quality relevant substances which originate from the various anthropogenic activities in catchments (e.g., agriculture, urbanization, sewage water treatment, atmospheric deposition, etc.). Such approaches have recently been undertaken by other groups, e.g., for nitrate (Basu et al. 2010) or urban pesticides (Rossi et al. 2013).

The Neckar catchments are embedded in a hilly topography between the foot of the Black Forest in the west and the Swabian Alb in the southeast. As part of the upper Neckar basin, they drain into River Rhine. Elevations range between 250 m a.s.l. at the outlet and almost 900 m a.s.l. in the crest of the Swabian Alb. From a geologic point of view, Middle Triassic limestones (Muschelkalk) crop out in the NW, followed in the southeastern direction by a sequence of evaporites and sandstones and claystones of the Upper Triassic (Keuper) and the Lower and Middle Jurassic. This progression is topped in the SE by the escarpment of the Swabian Alb consisting of Upper Jurassic limestones. The strata dip in the ESE direction is 1°–2°. Climatic boundary conditions are similar throughout the subcatchments with precipitation of 700–900 mm year⁻¹ and a yearly mean air temperature of 8 °C. However, the catchments differ strongly in land use (Table 1): The Goldersbach catchment (72 km²) is a primarily forested nature reserve with no industry, devoid of wastewater treatment plants or heavy traffic, which is in contrast to the neighboring Ammer catchment (134 km²) which is mostly agricultural and whose headwaters are located near the city of Herrenberg. The Steinlach and Echaz catchments show mixed land use, while the Körsch catchment is the most urbanized one, being situated just south of the city of Stuttgart and receiving treated wastewater from a series of larger sewage treatment plants. The selected catchments were screened with respect to existing data records and instrumentation, appropriateness for the various research questions, and accessibility, among others. Hydrochemistry of the catchments is hypothesized to reflect their land-use characteristics and geology (Schwientek et al. 2013a, b). Accordingly, the transport dynamics of nutrients and selected organic contaminants may be used to trace the dominating processes governing fluxes of water and matter (Selle et al. 2013). Groundwater – surface water interactions are studied at a test site along River Steinlach (Osenbrück et al. 2013).

Fig. 2 Locations of River Bode and Upper River Neckar test sites. For detailed maps of the River Bode test sites see Wollschläger et mult. (2013)



River Bode (Wollschläger et mult. 2013) is a tributary of River Saale within the Elbe basin. The Bode catchment covers an area of approximately 3,300 km². It extends from the Harz Mountains in its western part with elevations higher than 1,000 m a.s.l. down to the lowlands of the Magdeburger Börde in the east with elevations lower than 100 m a.s.l. The topographical bisectioning is reflected in geology, climate, and in land use: the mountainous part is characterized by Paleozoic granites, shales, and mudstones of differing degrees of metamorphosis, while the lowlands feature Triassic and Cretaceous limestones, sandstones and mudstones, partially covered with glacial deposits. Mean air temperature ranges from 5 to 9 °C, precipitation shows a variability between 1,500 mm/year in the mountains and less than 500 mm/year in the lowlands. Accordingly, the mountainous headwater regions of the Harz are primarily rural, forested areas compared to the intensively agriculturally used areas with fertile soils and higher urbanity in the Börde region. River Selke is a tributary of River Bode and drains a catchment of 456 km². Its area also shows the bisectioning characteristic of the whole Bode catchment with the mainly forested Harz Mountains in the southwest and agricultural lowland areas in the northeast. The long-term mean discharge at the gauge at Meisdorf is 1.5 m³ s⁻¹. Along an approximately 1 km long river section, a test site for studying stream-groundwater interactions was set up and complements the Steinlach test site. Research activities at the Selke site focus on the pattern and dynamics of water flow and solute transport within these morphological features. The Schäfertal experimental

catchment (Reinstorf et al. 2013) is a low-mountain catchment within the Selke catchment covering an area of 1.44 km². Land use is primarily agriculture along the hillslopes. The valley bottom is covered with pasture, whereas a small area in the very western part of the catchment is forested.

In addition to the own regional experimental activities, for land surface process studies data sets from eddy-covariance (EC) stations of the cooperating Research Unit FOR 1695 ‘Agricultural Landscapes under Global Climate Change—Processes and Feedbacks on a Regional Scale’ are available in WESS (<https://lsc.uni-hohenheim.de/91763?L=1>). These EC-stations are located at Kraichgau, an intensively used agricultural landscape, and at Central Swabian Alb, where crop lands are extensively used. Both research areas are peripheral to the Neckar catchment.

Understanding water and solute fluxes at catchment scale

Storage of water and solutes in catchments predominantly takes place in the subsurface. Water fluxes through the subsurface, however, are driven by boundary conditions which are affected by feedback mechanisms of the land surface–vegetation–atmosphere system. The interfaces at the land surface and between subsurface and surface water bodies play a crucial role for the determination of hydrological fluxes and travel times in the subsurface. The land surface-atmosphere interface and the river-groundwater

interface (hyporheic zone) are characterized by strong biogeochemical gradients. They potentially are particularly reactive zones, in which compounds are not only transferred between different environmental compartments and stored, but also chemically and/or biologically transformed.

In traditional compartmental analysis, the water, energy and matter fluxes across some of the compartmental boundaries have been treated as boundary conditions and were calibrated. Since these fluxes are particularly sensitive to environmental change, traditional compartmental models appear inadequate for projections of water resources quality under changing environmental conditions. The development and application of integrated models thus forms an important methodological focus. Additional methodological work packages on monitoring, modeling and measurement strategies lay the foundation of comprehensive and yet efficient analysis of catchments as complex systems in a changing environment.

Land surface-atmosphere interface and feedbacks

Climate models and hydrological models share the land surface as interface. Fluxes of water, energy and pollutants across this interface are predominantly governed by transport and turnover processes in the soil–vegetation continuum. Traditionally, water and solute fluxes in the single sub-systems (atmosphere, soil–vegetation and groundwater) are studied by separate models and the results of one class of models are transferred as forcing terms to the other classes of models. In order to achieve an advanced understanding of the impact of climate and land use change on exchange, transport, and feedback processes in the entire system, land-surface processes must be linked in a consistent way with the relevant processes in the atmosphere and subsurface compartments. Ideally, this should be done by complete coupling of regional climate models and meso-scale hydrological models via a land surface scheme with advanced biogeophysics. Improved simulations of the whole water cycle in the groundwater-land surface-atmosphere continuum allow providing information concerning its changes to decision makers and end users.

However, as the different types of models are acting at very different spatio-temporal scales, fundamental difficulties in data exchange between the components of such coupled model systems arise. Climate models generally do not provide sufficient spatial resolution to be used directly in hydrologic models. Whereas changes of soil and vegetation states can influence initiation of atmospheric convection, cloud formation and precipitation very rapidly, land-surface impacts on groundwater renewal take place at much longer time scales. The spatial and temporal distribution of groundwater recharge at regional scale is a key process for water and matter fluxes through catchments.

Quantifying this distribution is complex due to heterogeneities in precipitation and soil properties and due to the impact of seasonality of different vegetation types on evapotranspiration and infiltration.

To deal with different model resolutions, algorithms are needed for scaling down or up the exchanged variables and parameters to the respective resolution of the model to which the information is transmitted. Up- and down-scaling algorithms must account for flux conservation across the scales. Recent investigations show that the requiring flux conservation across different scales allows identifying averaging rules and thus effective parameters in spatially distributed mesoscale hydrological modeling (Samaniego et al. 2010). Simplifications in process representation, which are justifiable at one scale, may not be justifiable at a lower scale. As a consequence, oversimplifications in exchanged variables and parameters transfer inaccuracies from one model to the other. In case of the data transfer from climate models to hydrological models, inadequate downscaling can propagate to erroneous simulations of water fluxes and hence of other matter fluxes such as those of carbon, nitrogen, and environmental chemicals.

Moreover, due to deficits in hydrological components of climate models and their land surface schemes, using climate model output as input for hydrological models is still a challenge. Usually, climate models do not capture well the present climate variability and observed rainfall statistics at the regional scale. However, recent results show that errors in predicted rainfall statistics can be markedly reduced by increasing the resolution of atmospheric models. This has been demonstrated by the WWRP projects D-PHASE (Rotach et al. 2009) and COPS (Wulfmeyer et al. 2011). Particularly, extensive skill score analyses showed that future model runs should be performed on the convection-permitting scale (grid resolution <4 km) so that an error-prone approach can be omitted, the so-called convection parameterization (Bauer et al. 2011).

Incorporating more details of land-surface processes and orography in land-surface schemes apparently shows improvements in reproducing water and energy fluxes between land surface and atmosphere. This has been demonstrated in a variety of model systems, particularly the WRF-NOAH-MP model, which is one of the soil–vegetation–atmosphere model systems operated within WESS (Jiménez et al. 2012; Niu et al. 2012). For instance, short-range forecasts (Schwitalla et al. 2011) and regional climate downscaling (Warrach-Sagi et al. 2012), which are both very relevant for WESS, demonstrated considerable performance using the WRF-NOAH model. However, at the relevant scale of climate models, hydrological and canopy processes such as soil moisture distribution, crop growth and root water uptake are poorly represented in land surface schemes of atmospheric models (Ingwersen

et al. 2011). Crude parameterizations (e.g. rain interception), poor process resolutions (e.g. root water uptake), and missing processes (e.g. hydraulic redistribution) were identified to be responsible for deficiencies in the hydrological components of land surface models in simulating the water fluxes accurately (Bonan et al. 2011; Lawrence et al. 2011; Gayler et al. 2013). Inversely, hydrological and vegetation models at the smaller scale deliver information with feedbacks into climate models, as the water and energy balance at the land surface is closely linked to vegetation processes (e.g. seasonal dynamic of root and leaf development, physiological controls on transpiration) and soil moisture dynamics. It is meanwhile accepted that feedbacks exist between the subsurface compartments and the atmosphere (Maxwell et al. 2007; Maxwell and Kollet 2008; Ferguson and Maxwell 2010; Santanello et al. 2009) but implementation into models is basically absent. Patton et al. (2005) show in a numerical experiment that the development of convective cells in the atmospheric boundary layer directly relates to soil moisture patterns. Fluctuations in soil moisture and land-surface fluxes of water and energy subsequently feed back to the initiation of convection, cloud formation, and precipitation. Consequently, detailed descriptions and adequate parameterizations of these processes have to be incorporated in regional models because of their rather high impact on future projections of climate and matter cycles.

In summary, to bridge the scale gap between atmospheric and hydrologic models three complementary approaches are needed: (i) parameterization and realization of high-resolution regional climate projections up to the convection permitting scale to get a better understanding of feedbacks between soil/vegetation processes and the atmosphere, (ii) development of effective down- and up-scaling algorithms for the variables to be exchanged between models acting at different scales and (iii) incorporation of dynamic plant processes and physically more adequate process descriptions of water fluxes in the soil-plant-atmosphere continuum in land-surface schemes to get a consistent simulation of water fluxes from the atmosphere through the soil-vegetation continuum down to the groundwater (and back).

In the current phase, WESS concentrates on this long-term objective of a coherent link of land-surface processes with the relevant process in the atmosphere and groundwater compartments. In particular, we investigate which fluxes and state variables (and in which spatial and temporal resolution) have to be exchanged in a coupled atmosphere/land-surface model to adequately describe the impact of land-surface heterogeneities on fluxes between the soil-vegetation continuum and the atmosphere, but also on groundwater recharge at catchment scale and consequently as a function of land use and climate change. New concepts

of land-surface water flux simulation and parameter scaling are developed which are accompanied by a thorough verification activity based on existing data sets of water and energy fluxes across the land surface from cooperating research units (e.g. DFG Research Unit FOR 1695, see <https://lsc.uni-hohenheim.de/91763?L=1>, TERENO, Zacharias et al. 2011). Remote sensing data and campaigns are currently being prepared within the scope of WESS (Pause et al. 2013). First studies were performed to analyze the impact of different degrees of detail in models of root water uptake on simulated seasonal patterns of evapotranspiration and soil moisture at selected observatory sites in South Germany (Gayler et al. 2013; Wöhling et al. 2012b).

River-groundwater interface

To understand the hydrological functioning of a catchment, the water and solute fluxes from aquifers to rivers and vice versa are of great importance. The exchange of water between rivers, their bed (the so-called hyporheic zone), and the adjacent aquifer has strong implications on biogeochemical cycling, the fate and behavior of water-borne pollutants, and the net export of groundwater pollutants to rivers (e.g., Smith et al. 2009). Neither the dynamic behavior of these hyporheic exchange fluxes during hydrological events nor their spatial variability are well understood. To quantitatively assess net turnover within the hyporheic zone, not only water fluxes but also the key parameters controlling the associated reactive processes need to be estimated. This includes the travel time distribution of hyporheic exchange, its relation to biochemical transformations and the influence of a changing composition of the hyporheic sediment. The quantification of these parameters across scales requires the refinement of hyporheic zone monitoring techniques, the application of new, complementary tracer techniques, the development of suitable methods for mathematical analysis, and an improved process understanding using explorative, physically based numerical modeling experiments.

Monitoring of high spatial and temporal resolution—is it is required to study the relevant hyporheic processes—is usually limited to the bedform scale such as pool-riffle sequences, gravel bars, or meander loops (Kalbus et al. 2006; Fleckenstein et al. 2010). Within the WESS catchments, our hydraulic and biogeochemical monitoring activities focus on two newly established and well-instrumented sites at River Selke and River Steinlach (Osenbrück et al. 2013; Wollschläger et al. 2013). The magnitude and variability of hyporheic exchange fluxes is investigated using vertical gradients as well as continuous time series of hydraulic head, electrical conductivity, and water temperature (Schmidt et al. 2006; Anibas et al. 2009; Vogt et al. 2010a, b). Hydraulic properties and the

geometry of hyporheic sediments have been derived from surveys of streambed morphology, sediment texture, hydraulic testing and geoelectrical investigations (Doro et al. 2013). Time series of natural tracers like temperature, specific electrical conductivity, $\delta^{18}\text{O}$ of water, and dissolved ^{222}Rn are used to delineate travel time distributions of infiltrated surface water into the hyporheic zone (Cirpka et al. 2007; Osenbrück et al. 2013). Oxygen profiles using newly developed optode techniques (Haberer et al. 2011) and hydrochemical investigations including redox sensitive compounds and DOC provide information on transformations of organic matter and pollutants within the hyporheic zone. The associated metabolic rates as well as their interrelations with microbial community changes and functionality are studied using in situ microcosms and lab-based microcosm experiments (e.g. Febria et al. 2012).

Driven by the need to better understand the dependence of hyporheic reactivity on redox conditions and dissolved organic matter availability the aim is to establish and combine novel redox proxies with molecular-biological techniques in laboratory experiments and field investigations. The monitoring activities are complemented by 3-D numerical simulations of turbulent stream water flow (using OpenFOAM) coupled with flow and reactive transport in the hyporheic zone (using MIN3P). The modeling exercises aim to evaluate the impact of different boundary conditions on the coupled flow field and on biogeochemical reactions in the hyporheic zone using more realistic bedforms than in previous modeling studies (Cardenas 2009; Boano et al. 2010). Investigations beyond single bedforms require the application of integrating methods such as tracer experiments with natural or artificial tracers that address both the small scale and entire stream reaches (Gooseff et al. 2005; Cook et al. 2006). In order to better

assess hyporheic exchange flows we combined the conservative fluorescence tracer Na-fluorescein with the reactive fluorescence tracer resazurin. Resazurin has been shown to undergo irreversible reactions under biogeochemical conditions typical for the metabolically active hyporheic zone (Haggerty et al. 2008, 2009). The use of field fluorimeters for tracer detection allows to record the breakthrough curves of both tracers with a high temporal resolution (Lemke et al. 2013). The hyporheic exchange flux and the hyporheic travel time distribution are quantified by calibration of a 1-D advection dispersion model of in-stream tracer transport including hyporheic exchange using the measured breakthrough curves of the two tracers (Liao and Cirpka 2011). Figure 3 shows an example of a combined tracer experiment at a small stream within the Neckar catchment (for details see Lemke et al. 2012).

In future work, the findings on hyporheic exchange flow, transformations, and travel times will be integrated in a coupled stream-groundwater flow and reactive transport model driven by transient boundary conditions for a catchment-scale prediction of the fate of pollutants as is required for a reliable projection of river water quality.

Model calibration, uncertainty analysis, optimization of monitoring

Modeling complex environmental systems is challenging due to the non-linearity of the dominant flow and transport processes and the high degree of spatial and temporal heterogeneity. In addition, observations corresponding to state variables in the different model compartments, or to fluxes between these compartments, are typically scarce and their information content at the scale of interest is a priori unknown. To make predictions about future system

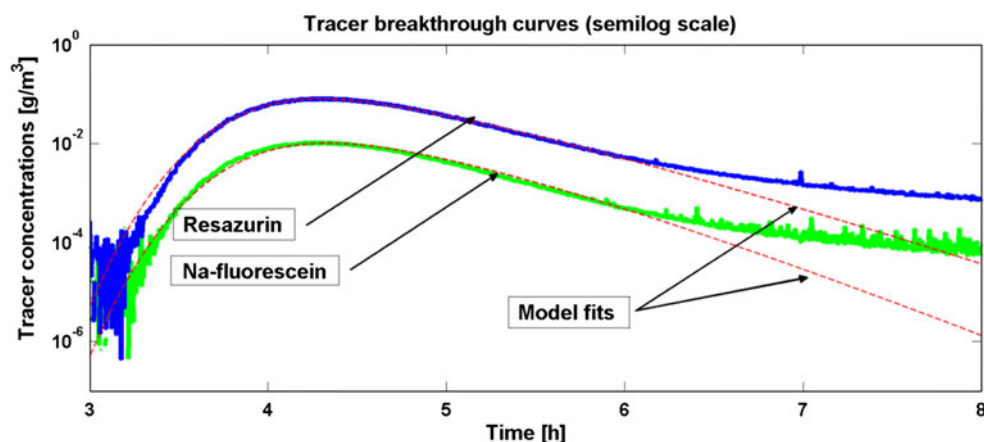


Fig. 3 Measured tracer breakthrough curves and joint model fit for the Goldersbach tracer experiment assuming an exponential travel time distribution (adapted from Lemke et al. 2012). A mass balance indicates loss of about 25 % of the reactive resazurin as compared to

conservative Na-fluorescein, suggesting a distinct hyporheic exchange. The fitted model indicates an exchange flow of 0.1 % of stream discharge per time unit with a mean travel time in the hyporheic zone of about 0.2 h

states with coupled system models, it is essential to calibrate model parameters that cannot be directly measured and to adequately treat uncertainties in the data (input, output, initial and boundary conditions) as well as in the model structure itself. The estimation of bias and uncertainty must be an integral part of any measurement, calibration or data assessment procedure. Otherwise, it is impossible to assess the quality of an analysis based on measured data. This requires a rigorous, model-based analysis of the measurement procedure and its conversion to the quantity of interest.

Different tools were developed and tested for model calibration, uncertainty analysis, and model-based optimization of monitoring strategies. We applied stochastic modeling techniques for multiobjective parameter estimation and uncertainty assessment of multi-layer vadose zone flow models (Wöhling and Vrugt 2011; Caldwell et al. 2012), a coupled surface–subsurface flow model (Köhne et al. 2011), dual-tracer, non-equilibrium mixing cell models for unsaturated bromide and chloride transport (Wöhling et al. 2012a), distributed hydrological models (Wöhling et al. 2013), and others (e.g. Nowak et al. 2012; Schöniger et al. 2012). These techniques are designed to be model-independent and for integration of different data types with arbitrary spatial and temporal resolution. Different (and partially contrasting) information of data about the environmental system can be revealed via efficient trade-off analysis approaches that utilize a multi-method optimization algorithm (Vrugt and Robinson 2007). These methods were applied as diagnostic tools to detect and reduce model structural deficiencies of coupled soil–plant–atmosphere models (c.f. Sect. “Land surface-atmosphere interface and feedbacks”) and to compare and evaluate multiple alternative model structures under consideration of the specific uncertainty of the individual data types (Wöhling and Vrugt 2011). The study by Wöhling et al. (2012b) revealed that the crop models SPASS and

GECROS with more detail in the process descriptions (e.g., for root water uptake) perform superior compared to the less detailed LEACHN and CERES models and that these models exhibit a much smaller trade-off between the simultaneous fit to soil water content, leaf-area index, and evapotranspiration data (Fig. 4).

An important source of uncertainty in integrated catchment models is the spatial parameterization of subsurface properties, which can not be determined at the required resolution by direct measurement methods. To address this issue, a soil–landscape model is developed to estimate the spatial structure of model parameters (e.g., water capacity and hydraulic conductivity). This structure is one of the most critical sources of uncertainty for modeling flow and transport in the heterogeneous subsurface. Our model approach aims to identify the spatial distribution of functional soil types at high resolution (10 m) which are associated with the parameters of interest. It is based on the approach of pedometrics augmented by geophysics and remote sensing. The resulting probabilistic parameter fields can be aggregated to the spatial discretization level that is utilized in integrated catchment models. This method merges point-scale information, spatially distributed indirect measurements and expert-knowledge to obtain improved a priori parameter fields of distributed subsurface properties and thus contributes to reduce the uncertainty of integrated catchment model predictions.

Another source of uncertainty with a particularly large contribution in coupled land-surface atmosphere models is the accurate and consistent initialization of land-surface and atmospheric variables. To improve the initial state of these models, research studies are ongoing to assess the impact of incorporating additional observations such as hyperspectral and SAR observations of the land-surface as well as of atmospheric variables using the global positioning system (GPS) and satellite radiances. Model imbalances and spin-up at initial time will be minimized by

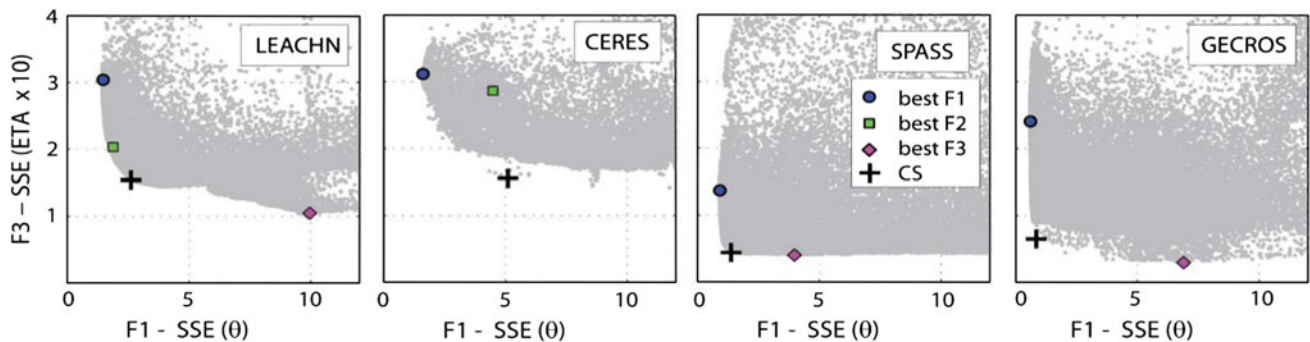


Fig. 4 Trade-off between the fits to volumetric water content and actual evapotranspiration of four coupled soil–plant–atmosphere models with different level of complexity. Less trade-off is observed with the SPASS and GECROS models, in which processes are

represented in more detail. F1, F2, and F3 signify the sum of squared errors (SSE) between measured and simulated soil water content, leaf-area index, and evapotranspiration, respectively. CS denotes an equally weighted compromise solution between F1, F2, and F3

sophisticated data assimilation (DA) techniques such as 3DVAR, 4DVAR or the Ensemble Kalman Filter (EnKF), by consistent and simultaneous assimilation of land-surface and atmospheric variables, and by digital filtering of atmospheric data at initial time. A first step in this direction is the setup of a probabilistic forecast system with ensemble-based DA (Warrach-Sagi and Wulfmeyer 2010, Grzeschik et al. 2012). The utilization of additional data sources improves model calibration, can help to preserve parsimony, and to reduce uncertainty. It has also a positive impact on initializing model states when atmospheric processes are modeled in the coupled system as demonstrated by Wulfmeyer et al. (2006), Grzeschik et al. (2008), and Schwitalla et al. (2011).

This call for ever more data is countered by the fact that catchment instrumentation, catchment-scale monitoring and field campaigns are notoriously expensive. Therefore, rational data acquisition techniques (called optimal design) are indispensable to feed the information needs of complex, coupled models. Especially under the combined conditions of model structural uncertainty, parameter uncertainty, and data that are noisy and scarce, optimal design is a promising approach. Starting from a geostatistical re-interpretation of classical optimal design theory (Nowak 2010), novel data collection optimization paradigms were developed for the situation of uncertain geostatistical model structure in Nowak et al. (2010). A related study (Nowak et al. 2012) looked at optimal data collection in order to support scientific or management decisions with maximum confidence. The approach follows the lines of Bayesian hypothesis testing for binary decisions, and optimizes the field investigation strategy to minimize the error probability (false positive, false negative) in the hypothesis test. The underlying statistical inference engine has to work with data values at planned locations that are not yet collected, which calls for a Monte-Carlo-like repetition of data assimilation with yet unknown, randomized, data values.

Leube et al. (2012) developed a method that can handle this situation in feasible time, without taking the usual linearized or Gaussian assumptions. However, coupled, highly parameterized large-scale models are often computationally very demanding. Model run-times that exceed hours or days prohibit a Monte-Carlo type analysis with the number of required repetitive model runs approaching and sometimes exceeding the order of 10^6 . For cases, where linearity assumptions are acceptable, we tested efficient predictive uncertainty estimation methods that require only a fraction of these model runs to evaluate and optimize monitoring networks (e.g. Moore et al. 2011).

Future research in this area will focus on (i) the development of improved techniques for converting indirect measurements (e.g. from geophysics and remote sensing) to the variables of interest (e.g. hydraulic subsurface

properties, soil moisture, etc.) while propagating the associated uncertainty of the measurement procedure and the conversion without relying on model linearization or assuming stationarity of processes, (ii) advanced data assimilation techniques as a key methodology for combining observations and models as well as for the optimization of parameters in coupled modeling systems, and (iii) improved methods of conditional statistics in general (e.g. Bayesian methods beyond Gaussian variables) that satisfy the efficiency requirements of computationally expensive integrated models (extending the work by Leube et al. 2012). Further, optimal design of field campaigns will be advanced towards the special feature of confident choice or weighting between alternative models in Bayesian Model Averaging.

Field measurements and monitoring: physical and chemical data

Numerous chemical compounds, which have been released into the environment by human activities, can nowadays be found everywhere, i.e. in the water, soil, and air compartments, at the poles and in high mountains, in other words globally (Daly and Wania 2005). Many of these compounds have reached a global distribution via the atmosphere; others have been applied to soils at regional scale by agriculture or released to groundwater locally from contaminated soils or by discharge of treated or untreated wastewater. Transport of these compounds is coupled to the water cycle—often via an intermediate storage in soils (Gocht et al. 2007). The crucial question for water quality is which of the numerous compounds have a potential to accumulate in the water cycle at what scale. This requires knowledge about the distribution of pollutants in the environment and a profound understanding of the dominant processes and flow paths determining water fluxes and storage and water driven transport and transformation processes within catchments (e.g. <http://www.cuahsi.org>, Barth et al. 2007).

For determination of water fluxes, monitoring requires a nested-scale approach reaching from mesoscale atmospheric observations based on advanced remote sensing systems, to basin-wide meteorological surveys using a combination of remote and in situ sensors (Behrendt et al. 2007, 2009), to hydrological studies at the scale of individual sub-catchments and detailed studies at the plot scale at hot spots of joint research activities (see Fig. 5). Within WESS airborne and satellite remote sensing activities are currently focusing on the WESS/TERENO reference site Schäferfalter (Table 1) where during April and October 2011 in total six flight campaigns were realized in cooperation with TERENO (Zacharias et al. 2011; Bogena et al. 2012)—specifically supported by the UFZ and the DLR

(German Aerospace Center). The campaigns made use of active microwave remote sensing using Synthetic Aperture Radar and imaging spectroscopy at different spatial scales. Key parameter fields of interest are surface soil moisture, soil texture characteristics of the shallow sub-surface, and vegetation conditions for distinct phenological stages of crop canopies. Data sets are complemented by satellite data as well as field-based activities as in situ sampling of soil moisture and vegetation parameters (Pause et al. 2012; Lausch et al. 2012).

Near-surface geophysical measurements provide the potential to non-invasively map and monitor soil properties (e.g., texture, soil depth) and state variables (e.g., water content, electrical conductivity) of the shallow subsurface at scales ranging from several m² up to a few km². Depending on the measurement setup and type of sensor applied, their integral depth of investigation ranges from a few decimeters down to several meters. Hence, their spectrum of application is manifold and highly valuable for hydrological applications: Geophysical measurements may be employed to either explore the very shallow subsurface and studying processes at the soil–plant–atmosphere

boundary or to investigate the deeper subsurface, e.g. the entire vadose zone down to the groundwater table as well as to characterize aquifer structures. In addition, time series of data measured at various system states allow for the estimation of water and solute dynamics at the intermediate scale of small watersheds or small basins (Robinson et al. 2008) which is hardly accessible with any other technique at the same resolution. Linking spatial geophysical measurements with hydrological processes is a rather young field of research. Much effort still needs to be spent to transform the information contained in measured proxy variables such as dielectric permittivity or apparent electrical conductivity into state variables such as water content in a way that they can be quantitatively integrated or assimilated into hydrological models.

Geophysical as well as soil properties and the related state variables can also be used as ground truth for remote sensing measurements (Pause et al. 2013) and for integration into different kinds of modeling studies, e.g., on hill-slope hydrology and soil landscape distribution. In the Schäferfalter catchment (Reinstorf et al. 2013), several electromagnetic induction (EMI) and gamma ray spectroscopy

Fig. 5 Monitoring strategies in catchments with relevant compartments (groundwater, soil, surface water, atmosphere) ranging from satellite and airborne observations to ground-based physical and chemical monitoring campaigns (taken from: DFG 2012)



measurement campaigns were carried out providing the spatial distribution of different geophysical parameters within the catchment. Time-lapse EMI surveys along a hillslope will be related to continuous water content measurements of a soil moisture monitoring network in order to optimize the application of EMI for estimating spatial water content dynamics.

Monitoring of chemical inventory in catchments is based on regular analysis of surface waters and groundwater. As rivers and creeks integrate over the whole catchment, a monthly sampling campaign was performed in the River Neckar and its tributaries from 2009 to 2011 at approximately 40 locations. Groundwater was sampled tri-monthly from major springs and groundwater wells (up to 28 locations) located within the catchments. More than 120 chemicals were considered, with an emphasis on organic trace pollutant concentrations (Schwientek et al. 2013a). Both, surface waters (streams) and springs contain information about the systems they discharge, the springs giving a more focused view on the groundwater systems. For selected compounds (ions, PAHs, trace pollutants, DOC, etc.) the campaigns will be continued and also transferred to the Bode catchments.

In combination with easy-to-measure physical quantities (e.g., turbidity) these lab-intensive chemical sampling and analysis campaigns also allow the identification of proxies. For example, a good linear relationship between total concentrations of PAHs in surface waters and the amount of suspended solids in the adjacent, but contrasting catchments in the River Neckar region was found, indicating particle-facilitated transport of PAHs. From these correlations, average contaminations of suspended particles were calculated, which can be considered as an integrated measure of sediment quality in the streams of these catchments. These concentrations differ in the different catchments and correlate well with their degree of urbanization taken as the number of inhabitants per total flux of suspended particles (Schwientek et al. 2013a; Rügner et al. 2013). Furthermore, concentrations of total suspended solids in water samples correlate very well with turbidity measurements over all catchments, indicating that on-line turbidity monitoring may be used to assess particle-associated fluxes of pollutants in streams at high temporal resolution.

Analysis of persistent pollutants and their distribution patterns in soils and river sediments—although complicated by strong spatial heterogeneity and variations in sediments quality—give insight into legacy pollution. For comparable rivers in SW-Germany (Ammer catchment) and China it could be shown that pollutant concentrations in sediments are higher in River Ammer, which most probably still reflects the long-lasting industrial history of European countries (Liu et al. 2013). Assessment of water quality of River Neckar and its tributaries is also based on

measurements of persistent and emerging pollutants in biota (e.g. fish) or using passive sampling devices (Martin et al. 2003)—whereby the development of suitable passive samplers makes up an own research task within WESS. First investigations confirmed the comparably high pollutant levels in the River Ammer (e.g. PAH, PCB) or Körsch catchments (Triclosan).

The dynamics of solute transport is studied based on novel on-line measurements in stream water. Therefore, several multi-parameter probes enabling high resolution monitoring of various quantities (discharge, nitrate and oxygen concentrations, electrical conductivity, pH, redox potential, turbidity) have been installed in chemically contrasting tributaries of the River Neckar as well as in the Bode catchment. For example, it was found that in the Neckar catchments average nitrate concentrations in stream water perfectly reflect the proportion of fertilized arable land (Ammer: 32 mg l⁻¹ vs. 47 %; Steinlach: 7.6 mg l⁻¹ vs. 11 %; Goldersbach: 3.2 mg l⁻¹ vs. 0.5 %). The dynamics of nitrogen transport, however, largely depends on the hydrologic system and is driven by the dominating runoff generation processes. The interplay between different hydrological storages, which eventually also act as N pools, turns out to be decisive for the temporal variability of N concentrations in stream discharge. Inversely, the study of N transport dynamics can be used to infer the hydrologic mechanisms responsible for N mobilization. In general, this helps to explain either chemostatic or dynamic behavior of whole catchment systems and gives insight into process patterns and which processes are relevant at the catchment-scale (Basu et al. 2010; Schwientek et al. 2013b). In addition, considering data records from previous projects reaching back to the 1970s and 1980s allows the identification of trends. The newly gained process understanding and the high resolution time series is used for the setup and improvement of process models (Selle et al. 2013). Finally, working in contrasting catchments allows to derive correlations (e.g. intensity of agricultural use vs. nitrate concentrations) and to use them for scenario simulations. The results highlight drivers of matter dynamics in river systems and will ultimately help to better understand and predict nutrient and contaminant budgets at the catchment scale. Ongoing work also addresses transport and transformation of pollutants from an ecosystem perspective, e.g. looking at distribution of organic compounds in sediments, suspended particulate organic matter including organic carbon and finally biota (e.g. fish).

Development, application and benchmarking of integrated models

Addressing the process-based research questions of complex catchments requires an integrated modeling strategy

due to the interaction and interdependencies of processes across the boundaries of environmental compartments. For models representing individual compartments, the spatial and temporal scales for the processes of interest differ significantly. Specifically, flow and transport state variables in the subsurface such as water levels or solute concentrations vary much slower but over shorter distances than typical atmospheric state variables such as air temperatures. Consequently, joint expertise of all disciplines is needed to develop an appropriate platform for integrated modeling of processes across compartmental boundaries.

In order to solve practical problems, continuous workflows are being established by executing the complete cycle for realistic model development including data management (Kunkel et al. 2013), pre- and postprocessing tools, simulation methods for coupled processes as well as data visualization (Rink et al. 2013) and validation strategies based on benchmarking (Kolditz et al. 2012). Currently the development of concepts for integrated hydrosystem analysis is a very active research field with the goal to improve the understanding of feedback processes between different environmental compartments such as the hydrosphere, pedosphere and atmosphere. A comprehensive overview on physics-based approaches can be found e.g. in Spanoudaki et al. (2009). For more recent developments we refer e.g. to HydroGeoSphere (Sudicky et al. 2008; Brunner and Simmons 2012), ParFlow (Maxwell et al. 2011) or CATHY (Sulis et al. 2011) to mention a few. In addition, open source initiatives, as for example the OpenGeoSys (OGS) project for modeling coupled thermo–hydro–mechanical–chemical (THMC) processes in porous–fractured media, are growing rapidly. Within OGS, partial differential equations are solved with Eulerian (finite elements, volumes, differences) and Lagrangian (e.g. random walk particle tracking) methods (Park et al. 2008). Recently, a compartment approach has been established to allow rapid coupling of hydrological compartments via exchange fluxes (Delfs et al. 2009). Hydrological processes between different compartments (river, soil, aquifer,

surface, etc.) are sequentially coupled, while processes within the same compartment (e.g. hydro-mechanical, dual-porosity, multi-phase flow) are coupled with global implicit schemes. A number of code coupling projects are completed, such as linking OGS to the Storm Water Management Model (SWMM) (Delfs et al. 2012), and to the Biochemical Reaction Network Simulator (BRNS) (Centler et al. 2010). Work in progress includes coupling OGS with the program package Expert-N which simulates water, nitrogen and carbon dynamics in the soil–plant–atmosphere system (e.g. Biernath et al. 2011). An overview of OGS couplings and interfaces can be found in Kalbacher et al. (2012).

Examples for the application of OGS for the simulation of hydrological processes are shown in the following based on the Ammer catchment in south-west Germany. The Ammer catchment is extensively used for groundwater production from a confined limestone aquifer and characterized by an above average proportion of agricultural (71 %) and urban (17 %) areas (Table 1). The Ammer River is mainly fed by groundwater springs coming from a partially karstified Triassic limestone aquifer (Upper Muschelkalk). In order to develop a realistic approach of the Ammer catchment several methods have been employed for both geometrical representation and processes studies for flow and reactive transport at different scales (Selle et al. 2013). Figure 6 (left) shows the realistic Ammer catchment model integrating information from different sources, i.e. digital elevation models (DEM, river network), geology (wellbore data, stratigraphy) as well as hydrology (groundwater levels, spring discharges).

As an important step towards a coupled model, a steady-state groundwater model was first calibrated against water levels and also compared to apparent groundwater ages estimated from concentrations of tritium and sulfur hexafluoride using a combined exponential-piston flow model with admixture of an ancient and tracer-free water component. The model application (Fig. 6, right) resulted in a better understanding of capture zones for the production

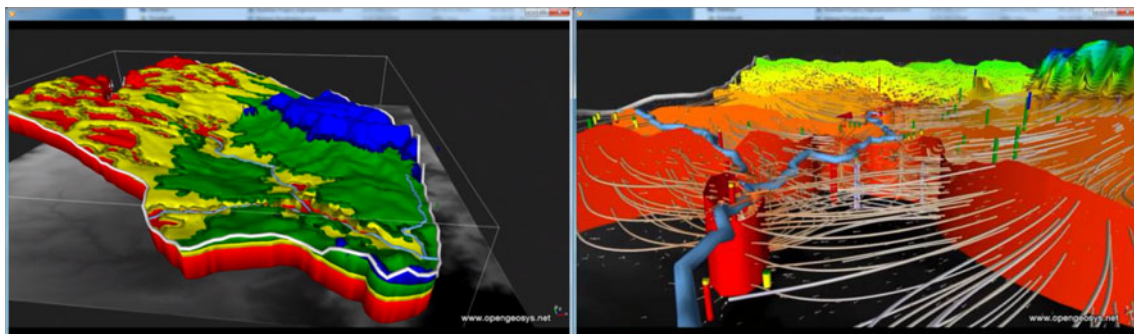


Fig. 6 The Ammer catchment: Geometrical representation (*left*) Groundwater flow model (including flowpaths to groundwater abstraction wells; *right*). Data visualization by Bilke (2012)

wells and the associated travel times of water to the wells (Selle et al. 2013).

In addition to catchment-scale groundwater studies, a hillslope model was developed to analyze reactive mass transport processes in the Ammer catchment. Using the OGS modeling platform, a coupled overland flow—Richards' flow model was set up. Details and a discussion of conceptual and numerical questions can be found in Delfs et al. (2013) and Maier et al. (2013).

As the availability of exact (analytical) solutions for coupled hydrosystems is limited to very basic/simple situations, benchmarking have to be developed for testing accuracy, reliability, validity, and predictability of numerical approaches. Benchmarking need to include a comparison of different modeling concepts such as conceptual and process-based approaches (as used in the above study).

Model inter-comparison initiatives have proven to be a valuable tool to increase confidence in model predictions and foster the cooperation between different developer teams (Sulis et al. 2010). Since there is a growing number of complex catchment models which seek to combine surface and subsurface flow, the international benchmarking initiative HM-INTERCOMP aims at a systematic inter-comparison of process-based models which coupled shallow water surface-Richards subsurface flow. Preliminary results of the first set of synthetic test cases exist. The more complicated examples of this set bring out some of the differences in physical process representations and numerical resolution approaches between the models. Currently, comprehensive benchmarking of the coupled models (some with heat and solute transport processes, feedbacks with atmosphere) requires more test cases including experimental data sets from lab scale to real-world catchments, e.g. from the contrasting catchment sites described in “[Contrasting catchments](#)”.

Outlook

Besides applying innovative monitoring and modeling technologies to gain basic research insights, WESS will expand to address socio-economic challenges and develop engineering solutions needed for water management at the appropriate scale which may comprise entire catchments, landscapes or basins. Comprehensive models of water flow and reactive solute transport are a prerequisite to assess costs and to quantify benefits of water management options in different scenarios for water providers, regulators and policy makers. WESS is already closely collaborating with drinking water providers, industry partners, industry associations, and environmental protection agencies and will provide the expertise from all relevant disciplines

(hydrology, geology, biochemistry, engineering, meteorology, etc.) needed for successful water management. First examples of bringing basic research results into applications are the safe exploitation of georesources (e.g. the operation of limestone quarries in groundwater recharge areas) or use of recycling materials in landscaping (e.g. in noise protection walls or in railway track and street dams), the assessment of risks from intensive agricultural activities (nitrate, pesticides) for local drinking water supply, and the evaluation of impacts of pollutants from urban areas on surface water quality.

Acknowledgments This work was supported by a grant from the Ministry of Science, Research and Arts of Baden-Württemberg (AZ Zu 33-721.3-2) and the Helmholtz Centre for Environmental Research—UFZ, Leipzig. Research in the Bode Catchment was in addition supported by TERENO (TERrestrial ENvironmental Observatories).

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