XXVIII. DoktorandInnen Treffen
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Organisatorinnen: Babette Gabriel & Theresa Frommen

DoktorandInnen-Treffen zum (inter-)nationalen Austausch an der Freien Universität Berlin

Am 7. und 8. Juni 2018 fand das XXVIII. DoktorandInnen-Treffen der Hydrogeologie an der Freien Universität Berlin statt. Der erste Tag war Exkursionen zu verschiedenen Themen der Berliner Wasserinfrastruktur gewidmet. Mit einer aufschlussreichen Führung durch die *Oberflächenwasseraufbereitungsanlage Tegel* und einer Besichtigung der *Baustelle zur Errichtung eines Stauraumkanals unter dem Mauerpark*, ermöglichten die Berliner Wasserbetriebe eine eindrucksvolle Exkursion für die rund 30 Teilnehmenden. Abschließend gab Prof. Dr. Michael Schneider an der Havel eine Einführung in die Hydrogeologie Berlins, mit Fokus auf die Uferfiltration.

Am zweiten Tag entstanden bei Vorträgen und Posterpräsentationen spannende Dialoge. Insgesamt diskutierten 30 Teilnehmende aus Deutschland, dem Iran und Kolumbien über Themen wie Geothermie, Grundwasser-Modellierung und Stoffumsetzungen, Küstenaquifere und Salzwasserintrusion, Charakterisierung und Modellierung der Sickerwasserbewegung anhand stabiler Isotope, Sulfat und Pestizide im Grundwasser, Abflussverhalten von Karstquellen im Iran sowie der Wasserinfrastruktur in Indien. Das Treffen in diesem Format fand großen Anklang da es den DoktorandInnen die Möglichkeit eines intensiven Austauschs gibt.

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Abstracts

Technical potential assessment of shallow geothermal groundwater resources – An application in the City of Munich

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In regional development, politics has integrated multiple actions for mitigation and adaptation of climate change into their agendas. Initiatives, like the Covenant of Mayors, encourage municipalities and cities to commit themselves towards ambitious targets of sustainable energy production. The actions to accomplish those targets mostly focus on renewable sources, which are established in municipal energy planning. The quantification of the shallow geothermal potential and especially the potential for the thermal use of groundwater is often neglected or only incidentally mentioned. This leads to a missing awareness of a highly capable and renewable energy source for heating and cooling.

A main reason for this situation is the lack of comprehensive concepts for the assessment of the geothermal potential (cf. Abesser, 2007). The thermal potential estimation for groundwater is subject to many different issues. Regulatory and operational constraints, but also complex well yield and thermal anomaly estimations, which depend on a wide variety of influential parameters. A major challenge for the assessment of the potential is the very different spatial knowledge about the hydrogeological influences. In an elaborated concept, the evaluation of input data of varying quality or spatial resolution should be possible by available uncertainty measures.

Within the EU-Interreg project GRETA, we develop a concept for the spatial assessment of the potential for the thermal use of groundwater that involves all relevant topics in a holistic approach (Casasso et al., 2017). Prior to a quantitative assessment, regulatory criteria like drinking water protection or temperature thresholds, as well as geotechnical constraints are reviewed. In the following step, the hydraulic potential, which corresponds to the maximum yield of a well doublet without hydraulic breakthrough, is quantified. The derived yield is used in the second step to estimate the size of the thermal anomaly. With the integration of a spatial character, areal queries lead to a reasonable technical potential where thermal interactions between neighboring users are avoided. By the consideration of the spatial impact of hydraulic and thermal changes, the method is suitable for energy planning in municipalities and cities. The essential dependencies are elaborated through exhaustive parameter variations in numerical box models. With the numerical approach, we assure that also complex non-linear coherences are represented.

The method is applied in the city area of Munich, where detailed raster maps are available for all relevant input parameters. Reports on existing systems are used for plausibility checks and a verification of the method. The work in the GRETA project is currently ongoing and the presented results are preliminary.

References

ABESSER, C. (2007): Open-loop ground source heat pumps and the groundwater systems: A literature review of current applications, regulations and problems. British Geological Survey Open Report, OR/10/045. 31pp.

CASASSO, A., PIGA, B. ,SETHI, R., PRESTOR, J., PESTOTNIK, S., BOTTIG, M., GOETZL, G., ZAMBELLI, P., D'ALONZO, V., VACCARO, R., CAPODAGLIO, P., OLMEDO, M., BAIETTO, A., MARAGNA, C., BOETTCHER, F., ZOSSEDER, K. (2017): The GRETA project: The contribution of near-surface geothermal energy for the energetic self-sufficiency of Alpine regions, Acque Sotterranee - Italian Journal of Groundwater, 6, DOI: 10.7343/as-2017-265.

Groundwater circulation cells for geothermal use: Preliminary results of the project Integralsonde Type II

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Groundwater heat pump (GWHP) systems are a widespread technique to provide buildings with heating and cooling. Most open loop shallow GWHPs are doublet systems which consist of two wells, one for extraction and one for reinjection of groundwater. Hence, there has to be enough space to set up such a system.

Shallow groundwater circulation wells (GCW) are an alternative. These open loop low-enthalpy shallow geothermal energy systems extract and inject groundwater in the same well via two filter screens at different depths. GCWs also demand less space, but so far there are only few installations. Our aim is to investigate the efficiency of those systems, their influence on groundwater chemistry and microbiology and evaluate their long-term productivity. These are the main research goals of the research project “Integralsonde type II” (01LY1507B /BMBF, KMU-innovativ). GCWs for geothermal use and their impact on groundwater quality are investigated at several sites in the quaternary main aquifer (Saalian age) in the Berlin (Germany) area. For the system studied, groundwater is extracted at the lower filter screen and pumped to a GWHP where the thermal energy is utilized for cooling or heating of the building and then reinjected via the upper well screen. The temperature gradient between extracted and injected groundwater is around 3 K. Since the groundwater circulates in the same aquifer which is used for drinking water production, it is crucial to avoid any negative impacts on groundwater. To reduce clogging, mineral precipitation, and dissolution, or physical processes such as particle mobilization, degassing and flocculation, it is critical to prevent mixing of different hydrochemical zones. Especially the presence of high contents of ferrous iron and manganese are usually exclusion criteria for the installation of open geothermal groundwater systems. We monitored both newly installed as well as running GCWs by sampling groundwater from the well and nearby groundwater observation wells. Major anions and cations, especially ferrous iron, manganese and sulfate as redox sensitive parameters, as well as physicochemical parameters for redox zone determination were analyzed. To monitor changes within microbial community, DNA from groundwater samples was extracted and used for quantitative real-time PCR applying primers for iron-reducers, -oxidizers and sulfate-reducing bacteria.

Our preliminary results showed that the redox zones in the vicinity of a newly installed GCW remained stable if groundwater was pumped in intermittent intervals. Continuous pumping over weeks changed the bacterial community of the produced water. A groundwater circulation well could therefore be a potential alternative for groundwater otherwise not suitable for open geothermal systems.

Decadal trajectories of nitrate input and output in three central German catchments with differing land uses

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Increased anthropogenic input of nitrogen to the biosphere during the last decades were followed by increased riverine concentrations of N (primarily as NO3-N) causing exceeded drinking water limits and eutrophication as a global problem. A better knowledge about the fate of N after its agricultural application is indispensable to understand recent and to project future trends of stream NO3-N concentrations. Contributing to this, we pursue two following research questions: Are there considerable time lags between in- and output, and by that a built-up of an N-legacy? And, are there dynamics in the output on decadal and seasonal time scales?

The selected catchment to answer these questions was the Holtemme catchment (269 km²) in Central Germany, which provides long-term data for many environmental variables including water quantity (e.g. precipitation, discharge) and water quality at various locations. This study compares the anthropogenic N-inputs from fertilizers and atmospheric deposition with riverine N-outputs over three decades in three nested catchments of the Holtemme. These subcatchments show the characteristic land use and topographic gradient from the upstream pristine mountainous conditions to intensively agriculturally used lowland downstream conditions near the outlet. The temporal and quantitative input-output assessment uses a time-series analysis on both intra- and inter-annual scales.

The comparison of N-input and -output at the outlet revealed a time shift of around ten years regarding measured flow-weighted annual concentration. Furthermore, the cumulated input from 1976 – 2015 was 42.758 t, while the riverine export of the catchment in the same time has been only one fifth of that. Consequently, we hypothesize that the significant storage of 88% N is either removed via denitrification or are still being stored within the terrestrial system as in the soil, groundwater and stream.

The intra-annual differentiation of concentrations shows the strong seasonality, but as well changing seasonality patterns over time. The latter is attributable to vertical N-migration to different aquifer depths over time and their changing contribution to the seasonal discharge. The vertical migration of N-input also results in changing concentration-discharge-relationships over the years, evolving systematically from accretion (increasing concentration with increasing discharge) over dilution (decreasing concentration with increasing discharge) to chemostatic (no change in concentration with changing discharge) behavior.

The study shows a strong changing chemical behavior over time and space that to a large extent is attributed to the agricultural input history and travel times to the stream, respectively. Hence, excessive anthropogenic N-input has on the one hand a long lasting effect on the catchment as a result of long travel times, and on the other hand a significant impact on the chemical conditions for the riverine ecosystem. Furthermore, up to now, at none of the three investigated stations, the strong decrease in N-input (after 80's) is followed by a comparable time shifted decrease in N-output. These constantly elevated concentrations in concert with the lack of 88%

of the N-input account for a high legacy effect of the catchment. Hence, although excessive application of N-surplus is prevented nowadays, the legacy from the last decades will impact the water quality also in the near future. Overall our study underlines the need for long-term management approaches to achieve the goals concerning water quality and to handle global eutrophication problems.

Transient effects of groundwater pumping on the 3D hydrothermal configuration of Berlin, Germany

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The major objective of this study is to understand the hydraulic and thermal state of the subsurface beneath the major urban center of Berlin, capital city of Germany. To achieve this goal, we implemented newly available hydrogeological data, which have been used to parametrize the 3D models of this study in space and time regarding hydraulic connectivity of surface water resources to the subsurface as well as groundwater extraction for supply purposes.

The model area is located in the Northeast German Basin and consists of a sequence of sedimentary deposits of several kilometers thickness. The sedimentary succession consists of alternating aquifers and aquitards deposited during Cenozoic times. This succession contains the freshwater aquifers that are used for municipal water supply. These are separated from the deeper saline aquifers by the local Oligocene Rupelian aquitard, which displays a heterogeneous thickness distribution due to glacial erosion, being discontinuous in some places.

Based on newly available data and aided by previous modelling studies, we found that leakage of deeper saline water through the main target aquifer is more widespread and not limited to places where the main aquitard sequence has been eroded. Pervasive leakage in and from the Rupelian aquitard (possibly leaching into the fresh water aquifer) is observed to occur also in areas where the clay layer is present in correlation with a relative strong component of hydraulic forcing from the surface.

We present results of both, the qualitative and quantitative effects of the modified hydrothermal setting of the different model scenarios, focusing on the effects of large-scale groundwater pumping.

Hydrogeology and water infrastructure of northeast Jaipur, India

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Identifizierung hydrogeochemischer Prozesse zur Charakterisierung relevanter Sulfatquellen in einem urbanen Grundwasserleiter - Berlin

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The deep groundwater in the Malm aquifer (Upper Jura) of the Bavarian Molasse Basin: Usage of environmental isotopes and hydrochemical analysis for a better understanding of deep geothermal reservoirs

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The deep groundwater which is hosted in the Malm aquifer (Upper Jura) of the Bavarian Molasse Basin has a great potential for geothermal energy usage. However, up to now there is only little understanding of the local, regional and supra-regional flow regimes and the reservoir of the Malm aquifer. This leads to the investigative analysis of the hydrochemical and isotopical composition of the geothermal water at several geothermal sites. The objective of the study project "IsoMol" funded by the Bavarian State Ministry of the Environment and Consumer Protection is to assemble geological, hydrological, isotopical, and geochemical information to develop a holistic understanding of this complex hydrogeological deep groundwater system.

The successful exploitation of the deep geothermal water in the Malm aquifer is associated with structural characteristics e.g. matrix, fault systems or karstic structures which influences the isotopical and hydrochemical fingerprint of the deep water as well as the hydraulic conditions. In this study, we try to use the isotopic fingerprint of the environmental isotopes to determine the origin and age of the deep groundwater, characterize different reservoirs and delineate local, regional or supra-regional flow systems. It is tried to answer open questions about the origin of major ions sodium and chloride in the water of the southern Molasse basin which are dominating the hydrochemistry in a calcium and magnesium carbonate aquifer with the stable water isotopes (δ18O, δD) as well as cutting-edge analytical tools of strontium (87Sr/86Sr) and noble gas helium (3He/4He) isotopes. Therefore, the environmental isotopes are used to identify the composition of the deep water as a mixture of several water types in the Malm aquifer: a) a recent meteoric fresh water; b) a fresh glacial meltwater with an isotopic composition depleted in δ18O and δD; c) an "extreme" water component enriched in δ18O and δD; and d) a very old water component.

In this study, new datasets from further geothermal sites in the greater Munich area are presented and integrated in the context of existing data from the Bavarian Molasse (Balderer (1990), Bertleff et al. (1993), Stichler (1997)). We would like to use this data to clarify three main questions: (1) fit these new data from the southern area of Munich to the current model presentation, (2) is it possible to recognize local, regions of regional and supra-regional flow systems and (3) are hydraulic boundary conditions also in the isotope composition of the waters shown.

References

Balderer, W.: Hydrogeologische Charakterisierung der Grundwasservorkommen innerhalb der Molasse der Nordostschweiz aufgrund von hydrochemischen und Isotopenuntersuchungen, *Steir. Beitr. z. Hydrogeologie*, **41**, (1990), 35-104.

Bertleff, B., Ellwanger, D., Szenkler, C., Eichinger, L., Trimborn, P. and Wolfendale, N.: Interpretation of Hydrochemical and Hydroisotopical Measurements on Paleogroundwaters in Oberschwaben, South German Alpine Foreland with Focus on Quarternary Geology, *Proceedings*, Isotope Techniques in the Study of Past and Current Environmental Changes in the Hydrosphere and the Atmosphere, IAEA, Vienna, (1993).

Stichler, W.: Isotopengehalte in Tiefengrundwässern aus Erdöl- und Erdgasbohrungen im süddeutschen Molassebecken, *Beiträge zur Hydrogeologie*, **48**, (1997), 81-88.

Quantitative approaches to optimize the multi-compartment concept and for a model-based risk management for bank filtration in hydraulic and hydrogeochemical heterogeneous aquifer systems

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River bank filtration is an important source of drinking water in Germany. Pathogenic bacteria and viruses can often be found in the groundwater, because of the short travel times in the subsurface and often high concentrations from wastewater and agriculture in surface waters. Depending on the properties of the porous media they can be removed from the mobile water phase during the transport through the subsurface. Currently the transport under dynamic field conditions is especially in connection with the inactivation of viruses still only inadequately researched and therefore difficult to predict. Aim of this project is to create a process-based model for the risk assessment of virus contamination in river bank filtration in hydraulic and hydrogeochemical heterogeneous aquifers. For this a multi scale approach is applied to determine the key processes and influences on the transport of viruses. The most important parameters for inactivation and sorption of viruses are identified and their influence quantified with controlled small-scale laboratory column experiments. The transport behavior under controlled but field typical conditions (e. g. flow velocity, sediment composition) is investigated with mesoscale laboratory column experiments (2 m). Finally, a 1-year monitoring campaign is conducted at the waterworks Flehe in Düsseldorf (Germany), where river bank filtration is used now for decades to produce drinking water, to evaluate the laboratory results under uncontrolled natural highly dynamic conditions. Based on a 2-dimensional model of the field site using a discrete as well as a geostatistical representation of the natural heterogeneity a monitoring and risk assessment concept will be developed to allow a more accurate prediction of virus transport in natural aquifer systems.

Compartment analysis to predict flood generation in a karst catchment

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A knowledge of key factors controlling runoff generation is vital for an effective flood warning, especially for karst catchments. However, runoff generation can be a very complex process involving a vast range of factors varying in space and time. Additionally, the knowledge of the size of surface water and subsurface catchments are crucial for a profound early warning system.

In order to better understand the system behavior of the Lauchert karst catchment in the Swabian Alb, SW Germany, we analyzed a wide range of data, including spatially distributed precipitation data, landuse information, soil properties, changes of soil water storage, groundwater level changes, hydraulic aquifer properties, results of tracer experiments, as well as spring discharge and stream runoff. A joint analysis of the data made it possible to delimit the catchment and identify compartments relevant for flood generation including their characterization.

It was possible to show that in most conditions runoff is generated only within the subsurface catchment. For modelling purposes, this is vital information, since the subsurface catchment differs significantly from the surface catchment in parts of the studied area. The data suggests further that runoff generation is largely controlled by the soil zone and the aquifer. Water storage in the soil, and flow through the unsaturated and saturated zone of the subsurface have the most important effect on the hydrograph of the river Lauchert. Even for high intensity rainfall events, the subsurface passage is the most important flow path.

Implications of different fault zone appearances on pressure signals in pumping tests for a typical setting of the Upper Jurassic deep geothermal reservoir in the South German Molasse Basin

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After the drilling and completion operations of a new geothermal well are finished, up to three acidifications in conjunction with short airlift pumping tests (a few hours) are generally applied in the Upper Jurassic deep geothermal reservoir of the South German Molasse Basin (Malm aquifer). At a later stage of the construction this is normally followed by a longer pumping test (up to several days) in which the pressure evolution in the geothermal well for stepwise increasing pumping rates is recorded. Those investigations are really important because they reveal if the exploration strategy was successful and if so how the reservoir is performing as well as what its hydraulic properties are. [Schneider and Thomas, 2012] To investigate the collected pressure data modern techniques are applied, which originated from the oil industry. For the evaluation of pumping tests, they get summarized under the term “pressure transient analysis” (PTA) [Houze et al., 2011]. A core method in PTA is the derivative analysis also called the Bourdet Derivative [Bourdet et al., 1983, Bourdet et al., 1989]. It allows for identification and quantification of well, reservoir and boundary models [Houze et al., 2011]. Ideally the effect of a fault on the pressure evolution can be seen in the Bourdet Derivative by its slope in the early time region (linear flow). The Malm aquifer shows in practice only rarely evidence for a flow regime around a geothermal well dominated by faults [Schneider and Thomas, 2012]. This doesn’t imply that there are no hydraulically active faults anywhere else at exploration sites in this aquifer. On one hand technical effects (e.g. well bore storage, effects due to the used pumping technique, skin) can cloud the pressure signal in the early time region. But additionally a specific contrast between a fault and the aquifer matrix is needed for the system to actually show linear flow in a pumping test. By performing parameter studies while observing the Bourdet Derivative the impact of possible fault zone and reservoir settings on pumping tests with respect to the Malm aquifer was investigated. Therefore, a representative but simplified, three-dimensional, numerical box model (one 70 degree inclined fault surrounded by 500 meter thick aquifer matrix, one vertical well, 3000m 1 depth of the reservoir top, 1000m fault length) was built usingMeshIT [Blöcher and Cacace, 2013] and Paraview [Ahrens et al., 2005]. By means of this box model multiple different hydraulic simulations of idealized pumping tests were executed. The simulation code MOOSE Framework [Gaston et al., 2009] with the complementary application GOLEM [Cacace and Jacquey, 2017] was used. The main parameters that were varied are the fault zone thickness, matrix and fault zone permeability as well as storage, distance between well and fault zone and production rates. To account for the variety of different parameter combinations a Monte Carlo analysis was realized by application of the RAVEN code [Alfonsi et al., 2017] on a HPC system (LRZ linux cluster).

References

[Ahrens et al., 2005] Ahrens, J., Geveci, B., and Law, C. (2005). ParaView: An End-User Tool for Large Data Visualization, Visualization Handbook. Elsevier.

[Alfonsi et al., 2017] Alfonsi, A., Rabiti, C., Mandelli, D., Cogliati, J., Wang, C., Talbot, P. W., Maljovec, D. P., and Smith, C. (2017). RAVEN Theory Manual and User Guide. Idaho National Laboratory.

[Blöcher and Cacace, 2013] Blöcher, G. and Cacace, M. (2013). MeshIt - A software for three dimensional geometric modelling of complex fractured geological systems. Computers and Geosciences.

[Bourdet et al., 1989] Bourdet, D., Ayoub, J., and Pirard, Y. (1989). Use of Pressure Derivative in Well Test Interpretation.

[Bourdet et al., 1983] Bourdet, D., Whittle, T., Douglas, A., and Pirard, Y. (1983). A new set of type cuves simplifies well test analysis.

[Cacace and Jacquey, 2017] Cacace, M. and Jacquey, A. B. (2017). Flexible parallel implicit modelling of coupled Thermal-Hydraulic-Mechanical processes in fractured rocks. Solid Earth Discussions, pages 1–33.

[Gaston et al., 2009] Gaston, D., Newman, C., Hansen, G., and Lebrun-grandi´e, D. (2009). MOOSE: A parallel computational framework for coupled systems of nonlinear equations. In International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009), volume 239, pages 1768–1778.

[Houze et al., 2011] Houze, O., Viturat, D., and Fjaere, O. S. (2011). Dynamic Data Analysis. KAPPA.

[Schneider and Thomas, 2012] Schneider, M. and Thomas, L. (2012). Verbundvorhaben: Wissenschaftliche und technische Grundlagen zur strukturgeologischen und hydrogeologischen Charakterisierung tiefer geothermisch genutzter Grundwasserleiter am Beispiel des süddeutschen Molassebeckens. *Endbericht–BMU Forschungsvorhaben*, page 237.

Occurrence, reaction and transport behavior of cadmium in groundwater

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According to the European Water Framework Directive, groundwater quality was evaluated in the European Union. The assessment of several groundwater bodies in Lower Saxony resulted in a “poor” chemical status due to elevated cadmium (Cd) concentrations. To identify sources, reactions and the transport behavior of Cd a research project was initiated as part of the action program of Lower Saxony. Cadmium is one of the most toxic and mobile elements in the environment and due to its physicochemical similarity it tends to substitute for Ca in chemical structures, leading to uptake and bioaccumulation by humans and animals.

There is a lack of information about the processes that control Cd concentration in groundwater and hence, there is need for a detailed study of its behavior. There are a multitude of natural and anthropogenic sources for elevated Cd in groundwater. The release from phosphate fertilizers is presumably the most important anthropogenic source. Cadmium also enters groundwater via atmospheric deposition and point sources such as landfills and mining activities. The mobility of Cd in an aquifer increases in the presence of oxygen and nitrate if it is associated with sulfide minerals, particularly pyrite. If associated with carbonate minerals, it can be released due to dissolution during a drop in pH.

The provided dataset of Lower Saxony included groundwater analyses from 6,200 wells. The investigation contained time series analyses, calculation of background values for Cd in groundwater, and classification of geochemical water types to identify presumably reasons for elevated Cd concentrations. Additionally, the dataset was connected with Cd contents in soil and deposition provided from permanent soil monitoring sites. To investigate Cd release at locations with elevated Cd concentrations in groundwater, sequential extractions and batch experiments with sediment and groundwater samples were conducted.

The mean background value of Cd in groundwater of marshlands and lowlands was 0.13 µg/L, which is approximately three times lower than the mean value of 0.36 µg/L observed in Pleistocene glacial deposits (Geesten). Elevated Cd concentrations in groundwater can be linked to water types with both, agricultural influences (mainly nitrate) and acidification. The conducted analyses did not show increased Cd contents in sediments and give no indications for significant anthropogenic Cd input. Therefore, it is assumed that the origin of Cd in groundwater is geogenic, however, its release is most likely induced by anthropogenic influences.

Degradation and transport behavior of veterinary pharmaceuticals in the saturated zone - Laboratory experiments on spatial heterogeneity

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Numerous scientific studies prove the presence of drug residues in the environment. The use of manure as organic fertilizer is known to be the main entry pathway for veterinary pharmaceuticals. The development of resistance genes is just one of various negative consequences potentially arising from their occurrence in the environment. However, in order to counteract the spread of these environmentally hazardous substances, one have to fill the existing knowledge gap with regard to those parameters that significantly influence the environmental behavior of these compounds.

A suitable method to investigate sorption and degradation of organic pollutants are column experiments. Under controlled laboratory conditions, the boundary conditions of the experiment, such as pH or temperature, can be varied accordingly. However, processes occurring in the environment cannot be adequately simulated and the transfer of results to the field scale still poses a challenge.

The aim of the study was to obtain detailed information on the degradation and transport behavior of veterinary pharmaceuticals in the saturated zone, considering spatial heterogeneity. Selected veterinary pharmaceuticals were investigated by means of five columns running in parallel. The one-meter long, undisturbed sediment cores came from three different locations in Lower Saxony and were operated under saturated conditions with a bottom-up flow direction. The experimental setup allowed depth-dependent sampling and, thus, concentration profiles along the core could be mapped. The target substances were analyzed by liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS). The results provide information about the (spatial) heterogeneity of sorption coefficients and degradation rate constants of the target substances.

Evaluating the effective parameters on variation of large karst springs discharge in Kermanshah Province

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‘‘Karst’’ refers to terrain with distinctive landforms and a largely subsurface drainage system, arising from the high solubility of certain rocks in natural waters (Karami 2002). Karst carbonate formations cover about 11% of Iran’s land area (185,000 km^2) and the Zagros range is 55% of the total karst carbonate in Iran (Raeisi 2002). The most important water resources in Zagros are karstic aquifers, which outcrop over 20 percent of the Zagros surface.

There are many karst springs (that is called “sarab” in the local lingo) in Kermanshah province (more than 200 springs). The mean annual discharge of these springs is good relatively (the average annual discharge some of them is up 3000 lit/s). They supply the total potable water of these province (more than 2 million people) and provide water for irrigation. In the past two decades, many of them have dried up completely or temporarily. Until now, these karst springs and their related aquifers have not been studied comprehensively.

Lack of understanding of the impact of climate change by taking into account the characteristics of the aquifer and uncontrolled exploitation of the aquifer has caused a lot of problems, including changes in groundwater flow, intense and irreversible decline water level and drying springs ultimately.

Therefore, the basic objective of this study is to use the physio-chemical parameters and isotopic analyses of the springs, along with the knowledge of local geology to characterize the springs and the aquifer functioning and to determine the factors controlling the composition of karst groundwater and evaluation of important karst spring behavior and effective factors on the variability of their discharge. Important questions are:

- What is the effect of climate change (the amount and type of precipitation) on springs discharge and their variability?
- What is role of the aquifer characteristics springs (karst development degree, size and shape of the aquifer) on springs discharge and their variability?
- What is the contribution of anthropogenic factors (extraction of karst, alluvial adjacent aquifer and other man-made structure) on springs discharge and their variability?

An investigation of anaerobic methane oxidation coupled with denitrification (n-damo) in freshwater using stable isotopes

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Flow and reactive transport modelling of a site contaminated with chlorinated hydrocarbons

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A contamination of chlorinated hydrocarbons close to a small river has been detected a couple of years ago. Since then it is being investigated and treated. That led to a lot of available data which could be used to understand the situation quite well. Performed measurements include groundwater monitoring in several observation wells, a pumping test, measurements of the sorbed concentrations in the soil and concentration measurements in the surface water and the riverbed. Some parts of the contaminated soil have been excavated and replaced by clean soil. This measure improved the situation but could not lead to a tolerable concentration in the groundwater. Several measurements revealed that the contamination migrated into the loam below the aquifer, which led to the development of a secondary contamination source. Now, further treatments seem to be very difficult as the contaminated area is much bigger as it was initially. A small river is located very close to the contamination, which does not show any increased concentrations so far. If naturally occurring conditions in the area are sufficient to decay the contaminants, Monitored Natural Attenuation (MNA) can be used as a remediation measure. However, it has to be proven that even in the future no contamination will reach the river. For the prediction, a reactive numerical model was built with the numerical software Visual Modflow and the implemented module RT3D. With this software package it is not only possible to calculate the decay of each present chlorinated hydrocarbon, but also the production of chlorinated hydrocarbons with a reduced number of chlorine atoms. This is especially important as vinyl chloride with only one chlorine atom is the most toxic one amongst the CHC's. For the calibration of the model, measured concentrations in observation wells were used. Additionally, temperature measurements in the riverbed sediments have been carried out to calculate the spatially and temporarily variable flux of groundwater into the surface water.

The results were confirmed with measured pore water pressures in mini-piezometers that are installed in different depths in the riverbed sediments. The calculated fluxes and measured vertical hydraulic gradients are also used in the numerical model as boundary conditions and calibration targets. The model shows, that the flow situation in the transition zone between ground- and surface water is very important for the fate of the contamination as well as the faster decay of the contaminants in that zone due to a constant supply of oxygen and organic matter. Without assuming a stronger decay and an enlarged flow path it is hardly possible to calculate a concentration below the detection limit in the surface water body even if dissolution is considered. The case study offers a lot of interesting aspects regarding the handling of groundwater contaminations in the practice. Even the actually widely investigated research fields of groundwater and surface water interaction and diffusion into low permeable aquitards are included here. The development of the case, the results of the numerical model and planned measures will be presented.

References

Conant, Brewster; Cherry, John A.; Gillham, Robert W. (2004): A PCE groundwater plume discharging to a river: influence of the streambed and near-river zone on contaminant distributions. In: Journal of Contaminant Hydrology 73 (1-4), S. 249–279. DOI: 10.1016/j.jconhyd.2004.04.001.

Schmidt, C.; Bayer-Raich, M.; Schirmer, M. (2006): Characterization of spatial heterogeneity of groundwater-stream water interactions using multiple depth streambed temperature measurements at the reach scale. In: Hydrology and Earth System Sciences 10 (6), S. 849–859

Building a large-scale numerical model for modeling saltwater intrusion in North-Western Germany

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The area under investigation is located in North-Western Germany bordering the North Sea in the north and two estuaries, Weser and Ems, in the east and west. Throughout history inundation events have salinized groundwater and human have built dikes and installed drainage measurements to cultivate the land. To investigate the movement of the saltwater-freshwater interface these factors have to be taken into account for. A large-scale numerical model was built with a 500 m discretization in x- and y-direction and a vertical extent of 240 m discretized into 2 m thick computational layers. The geological structure was roughly incorporated by hydrogeological conductivities. All measurements integrated into the model (e.g. hydrogeological structure, chloride concentration, river levels, wells and drawdowns) have been provided by civil services and water supply companies. Real piezometric heads were used to validate the model to then replicate the current extent of salinization. Future scenarios will be implemented to forecast the interfaces movement and to factor in climate change.

Water flow characterization in the unsaturated zone using stable water isotopes and modeling

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A first step in gaining knowledge on pesticide fate in the subsurface is characterizing water flow processes. This can be done by using stable water isotopes (δ^2H, $\delta^{18}O$) as natural tracers in combination with modeling. In this study, two lysimeters installed in Wielenbach, Germany, were considered: Lysimeter 1 is filled with sandy gravels, and Lysimeter 2 is filled with clayey-sandy silts. Maize was cultivated at the site and pesticides (metolachlor, terbuthylazine, nicosulfuron, prosulfuron) were applied once a year. We have been measuring $\delta^{18}O$ and δ^2H in precipitation and in the lysimeter outflow water for 3 years. We used different lumped-parameter model approaches (LPM) considering transport through the soil matrix (advection and dispersion) and along preferential flow paths (piston flow) with different assumptions concerning evapotranspiration. Aims were to determine mean transit times of water (MTT), dispersion parameters (P_D) and the contribution of preferential flow for the different soils.

As preliminary results for water flow characterization, estimated MTT and PD were higher for silt (MTT of 362 d, PD of 0.7) than for gravel (MTT of 129 d, PD of 0.12). Small pores dominate in silt soils, which may lead to slower water movement (higher transit time) and a higher tortuosity (increased dispersion) as compared to the gravel soil. Consideration of preferential flow (13% for gravel, 10% for silt) could describe the flow processes in both lysimeters more adequately. Currently, we are comparing different estimations for the input function and evapotranspiration by considering (a) the water balance and weight of the lysimeters and (b) the Penman-Monteith approach. We will extend our study by numerical modeling (Hydrus 1D) for verifying the LPM approaches and obtaining further insights into water flow dynamics and the distribution of water content in the subsurface.

Modelling the formation and development of caverns in rock salt

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In Germany, salt deposits play an important role as industrial raw material as well as for energy storage. However, in case of a geological interference zone rock salt comes into contact with groundwater which may lead to the formation of geogenic caverns representing high risk to active potash and rock salt mining. In such cases, fluids migrate through fissures into the salt and start dissolving it subsequently leading to decompaction of the rock mass which may end up in subsidence of overlying structures. Therefore, damages at the surface as well as for the mine structures may result. The main aim of the project “ProSalz” is to improve the process understanding of reactive multi-phase flow in the transition zone between caverns and solid rock in order to facilitate a safe long-term retention of caverns within rock salt.

The Fluid Systems Modelling Section is responsible for the numerical simulations as well as the data management of the project. The aim of my doctoral thesis is to create several models on different spatial scales and to perform sensitivity analyzes within the parameter space of geochemistry and hydromechanics in order to support the conceptualization of laboratory and field experiments. Using data from laboratory measurements will finally help me to create more complex models and to calibrate them, so the chemical as well as the hydromechanical behavior of the caverns can be modeled and the mechanical stability can be evaluated.

So far, base models of all laboratory and field experiments have been created and different scenarios tested. The results provide important information about geometry, pressure and chemical composition of fluids to help design the experiments. While the dissolution process of salt is very fast, some transport mechanisms were shown to be too slow and therefore not relevant within the time frame of the project. Furthermore, the dissolution process along geological faults (cracks or fissures) in rock salt has been modelled in order to verify an existing approach that describes the development of natural caverns. The results significantly depend on the NaCl-concentration and the fluid velocity. All in all, the models quantify the geochemistry very well but not the hydromechanics yet. So far the geometry is highly simplified. Therefore, the next step is to improve the base models by using Navier-Stokes equations instead of Darcy´s Law and to model natural cavern systems of higher complexity. Available measurement data will be compared to the results in order to calibrate them. The final step after geochemistry and hydromechanics are implemented is to model the mechanical behavior of rock salt in order to evaluate the long-term stability of natural and technical caverns.

Understanding DOC mobilization dynamics through high frequency measurements in a headwater catchment

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Increasing dissolved organic carbon (DOC) exports from headwater catchments impact the quality of downstream waters and pose challenges to water supply. The importance of riparian zones for DOC export from catchments in humid, temperate climates has generally been acknowledged, but the hydrological controls and biogeochemical factors that govern mobilization of DOC from riparian zones remain elusive. By analyzing high-frequency time series of UV-VIS based water quality we therefore aim at a better understanding on temporal dynamics of DOC mobilization and exports. In a first step a one-year high frequency (15 minutes) data set from a headwater catchment in the Harz Mountains (Germany) was systematically analyzed for event-based patterns in DOC concentrations. Here, a simplistic linear model was generated to explain DOC concentration level and variability in the stream. Furthermore, spectral (e.g. slopes and $SUVA_{254}$) and molecular (FT-ICR-MS) characterization of DOC was used to fingerprint in-stream DOC during events. Continuous DOC concentrations were best predicted (R^2, NSE = 0.53) by instantaneous discharge (Q) and antecede wetness conditions of the last 30 days (AWC_{30} = $Precip._{30}/PET_{30}$) as well as mean air temperature (T_{mean30}) and mean discharge (Q_{mean30}) of the preceding 30 days. Analyses of 36 events revealed seasonal trends for the slope, intercept and R^2 of linear log(DOC)-log(Q) regressions that can be best explained by the mean air temperature of the preceding 15 days. Continuously available optical DOC quality parameters $SUVA_{254}$ and spectral slope (275 nm – 295 nm) systematically changed with shifts in discharge and in DOC concentration. This is underlined by selected FT-ICR-MS measurements indicating higher DOC aromaticity and oxygen content at high flow conditions. The change of DOC quality parameters during events indicate a shift in the activated source zones: DOC with a different quality was mobilized during high flow conditions when higher groundwater levels connected formerly disconnected DOC source zones to the stream. We conclude that the high concentration variability of DOC can be explained by a few controlling variables only. These variables can be linked to event-based DOC source activation and more seasonal controls of DOC production.