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Seasonality of temperatures and redox zonations during bank filtration – A modeling approach

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SUMMARY

Bank filtration (BF) is a common technique for supplying drinking water, using the ability of the infiltration zone and aquifer passage to attenuate or degrade undesired substances that infiltrate from surface waters to groundwater abstraction wells. Temporal and spatial changes of temperatures and redox conditions are often the controlling factors for the fate and behavior of micropollutants during subsurface passage and consequently for the extracted raw water quality. A 2-dimensional cross-sectional heat transport and multi-species reactive transport model was set up to simulate the seasonally varying temperatures and redox conditions on the infiltration path at a bank filtration site in Berlin, Germany. The calibrated model was able to capture the observed variations in O_2 and NO_3^- when considering temperature dependence of the redox reaction kinetics. The observed Mn^{2+}- and Fe^{2+}-concentrations were not well replicated by the model, presumably due to mineral reactions that were not accounted for in the simulations. SO_4^{2-} was found to behave conservative, i.e., the observed concentration could be well simulated without any reactions. The simulations reveal the transience of BF systems with regard to temperatures and redox conditions, which has important implications for the BF quality and should therefore be accounted for.

1. Introduction

Bank Filtration (BF) is a conventional technique to achieve a better groundwater/drinking water quality (e.g. Huntscha et al., 2013). Because of its high efficiency, this convenient technique has been widely used in Europe for more than a century (Hiscock and Grischek, 2002). BF can take place under natural conditions or be induced by pumping of surface water into the groundwater body (Hiscock and Grischek, 2002; Sharma et al., 2012). The conditions at the infiltration zone generally lead to a qualitative improvement of the bank filtrate by biogeochemical processes like sorption, ion exchange or biodegradation, removing, for example, nutrients, organic carbon and pathogenic viruses and bacteria that are often present in the surface water (Hiscock and Grischek, 2002).

Especially the ongoing reduction/oxidation (redox) processes chemically affect the water quality in aquifer systems (McMahon and Chapelle, 2008). These microbially mediated processes couple the most efficient electron acceptors to the most efficient electron donators. The most common electron donors in aquatic environments are dissolved (McMahon and Chapelle, 2008) and particulate (Hamersley and Howes, 2002) organic carbon (DOC, POC). With the influx of dissolved organic carbon via the infiltrating surface water at BF sites, as well as sediment-bound organic matter (SOM), the microbial activity is the driving force to exhaust the supply of O_2 and NO_3^-, followed by the reductive dissolution of MnO_2- and $Fe(OH)_3$-oxides (Berner, 1980). The order of redox sequences usually follows the availability of the most energetically favorable naturally electron acceptor. For instance, in aerobic aquifers, microbes gain the most energy from the reduction of O_2. If O_2 is depleted NO_3^- becomes the next most favorable electron acceptor. Thus, distinct redox zones form that are sequentially aligned along the flow path, i.e., starting with the aerobic zone (O_2-reducing), followed by the NO_3^--, MnO_2- and $Fe(OH)_3$-reducing, sulfidic and methanogenic zones (Hunter et al., 1998; McMahon and Chapelle, 2008).

As is generally known, redox processes directly affect the water composition. Besides they also have been found to be critically important for the removal efficiency of a number of trace organic pollutants in BF settings (Schwarzenbach et al., 1993; Greskowiak et al., 2006; Massmann et al., 2006, 2008b; Heberer et al., 2008; Banzhaf et al., 2012; Burke et al., 2014a,b).

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Bank filtration becomes increasingly important for drinking water production due to its natural ability to remove nutrients, organic carbon, and microbes, especially pathogens, present in the source water (Farnsworth and Hering, 2011). Hence there is a strong need for further investigation of the coupled physical and hydrobiogeochemical processes under highly transient hydrological and hydrochemical boundary conditions typically present at BF sites. The microbial activity and thus the consumption rate of electron acceptors depend on the availability of electron donors such as DOC/POC and also on the variations in the water temperature (Atlas and Bartha, 1998).

It was found in a number of studies that seasonal temperature changes of the infiltration water leads to a dynamic development and extent of redox zones during subsurface passage (Doussan et al., 1997; Prommer and Stuyfzand, 2005; Massmann et al., 2006, 2008a; Greskowiak et al., 2006; MacQuarrie and Al, 2008; Sharma et al., 2012). Thus, understanding and quantifying the redox dynamics and the resulting water quality during BF requires a comprehensive modeling framework comprising detailed descriptions of the transient flow and hydrochemical boundary conditions as well as appropriate reaction networks (Farnsworth and Hering, 2011), including the effect of temperature. However, to date there are only a limited number of modeling studies that account for this full range of effects during BF (MacQuarrie and Al, 2008; Sharma et al., 2012) or related infiltration ponds (Greskowiak et al., 2006; Vandenbohede et al., 2013) at operational scale.

Sharma et al. (2012) simulated dynamically changing hydrochemical processes at a RBF site at the river Rhine with a simulation period of 516 days and an average subsurface residence time of around 50 days. MacQuarrie and Al (2008) presented simulation results based on three measurements from July to September 2003. They intensively discussed the seasonal temperature change influencing the Mn^{2+} concentrations. Vandenbohede et al. (2013) simulated heat transport and its effect on the hydrogeochemical conditions during ponded infiltration in The Netherlands. The focus of that study was the long-term evolution of the major ion chemistry on the infiltration path as a result of seasonal temperature changes rather than a detailed replication of the seasonal redox dynamics. Similarly, Greskowiak et al. (2006) modeled heat transport and its effect on the hydrogeochemical conditions during ponded infiltration in Germany. The focus was on describing the observed redox dynamics in the aquifer dependent on the seasonal temperature changes. For both of the studied pond infiltration systems the average residence time was less than 60 days.

The present study adds to the limited number of existing comprehensive modeling studies on bank filtration and aimed at investigating the effect of seasonal temperature changes on redox zoning at a BF site at Lake Tegel in Berlin, Germany via reactive transport modeling. The main focus herein was on the temperature dependent simulation of O_2- and NO_3^--reduction, as the presence of O_2 and NO_3^- in particular appears to be the key control for the attenuation of various organic trace pollutants (Bradley et al., 2002; Gruenheid et al., 2005; Greskowiak et al., 2006; Massmann et al., 2008a; Baumgarten et al., 2011; Maeng et al., 2011; Banzhaf et al., 2012; Burke et al., 2014a,b). The developed model utilizes a data set of a three year study named NASRI (Natural and Artificial Systems for Recharge and Infiltration), which was conducted in Berlin from 2002 to 2005 (e.g. Massmann et al., 2006) and is one of the most comprehensive data sets recorded for BF sites to date. The data set still is used in several studies, due to its continuous stream of data for an enormous quantity and quality of parameters and emerging organic compounds. The reactive transport model is based on a previous model of this particular field site incorporating conservative transport of stable isotopes as well as first-order degradation of several organic micropollutants detected at the BF site (Henzler et al., 2014).

2. Materials and methods

2.1. Study site

The study area is located in the north west of Berlin where a well field of the Berlin Water Company (Berliner Wasserbetriebe, BWB) induces bank filtration at the western shore of Lake Tegel, a part of the River Havel. This study focuses on a transect of observation wells situated between Lake Tegel and an abstraction well (well 13, Fig. 1).

BF at the study site occurs in the Quaternary aquifer which is partly divided into an upper and lower aquifer by a glacial till layer located at a depth between 12 and 20 m. The hydraulic conductivities of both aquifers range between 1.1×10^{-3} to 6.0×10^{-4} m/s, with a mean value of 3.0×10^{-4} m/s. The hydraulic conductivities of the aquitard lie between 2.0×10^{-7} and 3.0×10^{-9} m/s (Wiese and Nützmann, 2011). Nevertheless, the upper and the lower aquifer are hydraulically connected due to geological windows in the aquitard (Wiese and Nuetzmann, 2009). Therefore, in the 2D cross-section model, the aquitard was assumed to be only slightly less impermeable with a hydraulic conductivity of 1.0×10^{-5} m/s.

Lake Tegel has a maximum depth of 14 m and the deeper parts of the lake are filled with impermeable limnic sediments restricting infiltration to the shore areas. The mean lake level varies from 31.3 m to 31.5 m above sea level (asl) between summer and winter.

With 0.02–0.08 weight% (mean value 0.04 weight%), the SOM content of the aquifer is low. The surface water contains a considerable amount of treated waste water (WW) due to the discharge of treated WW from a local wastewater treatment plant (WWTP) into the lake (Massmann et al., 2004a).

Physico-chemical properties and groundwater chemistry, including O_2, NO_3^-, Mn^{2+}, Fe^{2+} and SO_4^{2-}, were measured monthly between spring 2001 and autumn 2004 in the lake, all observation wells (Fig. 1) and abstraction well 13 to characterize the seasonally varying redox conditions during bank filtration.

The study transect has been the subject of a number of papers, mostly from the NASRI project. Heberer and Adam (2004) and Heberer et al. (2004) analyzed the fate and behavior of pharmaceutical residues. Furthermore, bulk dissolved organic carbon and some trace organic compounds were studied by Gruenheid et al. (2005) and Massmann et al. (2004a, 2008c) evaluated environmental tracer data. Massmann and Sueltenfuß (2008) investigated on excess air utilizing noble gas analysis. Wiese and Nuetzmann (2009) and Wiese and Nützmann (2011) performed hydraulic investigations. Sulfonamides and psychoactive compounds were studied by Richter et al. (2008) and Hass et al. (2012) respectively. Wiese et al. (2011) carried out a statistical analysis of NASRI data on organic micropollutants. Most recently, Henzler et al. (2014) modeled the transport of stable isotopes ($\delta^{18}O$ and δD) and the simplified reactive transport of organic micropollutants originating from WW, using the same model set-up presented herein.

2.2. Modeling of transient groundwater flow, heat- and reactive transport

In the present study we extended the existing flow and transport model of Henzler et al. (2014) of the site for heat transport and the temperature dependent microbially mediated terminal electron acceptor processes aerobic respiration, nitrate reduction, MnO_2- and $Fe(OH)_3$-reduction. The aim was to simulate seasonally