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# Reactive transport model for predicting arsenic transport in groundwater system in Datong Basin



Qian Yu<sup>a,b,\*</sup>, Yanxin Wang<sup>a,\*\*</sup>, Xianjun Xie<sup>a</sup>, Matthew Currell<sup>c</sup>

a State Key Laboratory of Biogeology and Environmental Geology, School of Environmental Studies, China University of Geosciences, 430074 Wuhan, China

<sup>b</sup> College of Resources and Environmental Science, South-central University for Nationalities, 430074 Wuhan, China

<sup>c</sup> School of Civil, Environmental and Chemical Engineering, RMIT University, Melbourne

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#### ABSTRACT

High As concentration in groundwater of Datong Basin has emerged as an issue of great concern in the past decade because of its serious impact on the health of many people. The present study is to our knowledge the first attempt model the transport of arsenic in this system using a 1D reactive transport model (PHREEQC). Based on published field data from Shanyin Field Site (Datong Basin), the importance of the (bio)geochemical processes for arsenic mobility is evaluated quantitatively using geochemical models of growing complexity. Arsenic mobility during the surface water and groundwater interactions can be explained by the reductive dissolution of iron oxyhydroxides, sulfate, nitrate and arsenate, and by surface sorption/de-sorption occurring in response to changes in geochemical conditions. Both the Fe(III) surface complexation model and the 1D reactive transport model were employed to depict the arsenic transport in shallow groundwater system during the surface water groundwater interactions for Well 1-2S and Well 2-2S, respectively, reflecting the important role of surface sorption processes on arsenic transport. The 1D model results revealed that redox processes were also critical. The improved calibration of model simulations involving both of these components indicates that the combination of processes is critical to understanding and characterising the transport of arsenic in groundwater during groundwater surface water interaction, especially close to the surface water body.

#### 1. Introduction

High arsenic groundwater is widespread in China's Datong Basin and has caused serious endemic poisoning of local residents due to longterm consumption of high arsenic groundwater (Li et al., 2005). To mitigate the arsenic risk and ensure a safe groundwater supply under these conditions, a full understanding of the arsenic enrichment mechanism in the Datong Basin groundwater is urgently needed, particularly any variations that occur during periods of irrigation or surface water-groundwater interaction (e.g. Yu et al., 2015). The most widely accepted mechanisms causing high aqueous arsenic concentrations in Datong groundwater are microbial reduction of Fe(III) complexes (Xie et al., 2013) and de-sorption of As from clay minerals and colloids driven by elevated pH (e.g. during carbonate weathering) and competitive sorption (Xie et al., 2008b; Guo et al., 2003). A major unresolved problem concerning the arsenic contamination of groundwater in Datong Basin, concerns the arsenic mobilization during the surface watergroundwater interactions and/or irrigation. Several explanations for

the arsenic mobilization during surface water-groundwater interactions and/or irrigation have been put forward. Yu et al. (2015) used stable isotopes (H and O) and strontium isotopes to verify that extensive mixing of surface water and groundwater took place during short-term artificial flooding. Arsenic contents fluctuated significantly before and after the flooding, which may be associated with the reductive dissolution of iron oxyhydroxides and sulfate stimulated by the surface water infiltration. Xie et al. (2015) also coupled water chemistry and geochemical modeling to investigate arsenic mobilization during irrigation and non-irrigation periods in shallow groundwater in the Datong Basin. Their geochemical inverse modeling results indicated that Fe oxide/hydroxide and Fe sulfide dissolution as well as siderite precipitation were the dominant processes related to the mobilization of arsenic from the pre-irrigation to irrigation period. However, they did not distinguish the principal geochemical processes controlling arsenic mobilization during these periods of transient surface water-groundwater interaction, that is pure Fe(III) adsorption, or pure redox reaction or a combination of the two. This paper focuses on clarifying the most

\* Correspondence to: Q. Yu, College of Resources and Environmental Science, South-central University for Nationalities, 430074 Wuhan, China. \*\* Corresponding author.

E-mail addresses: yuqian0811@yahoo.com (Q. Yu), yx.wang@cug.edu.cn (Y. Wang).

https://doi.org/10.1016/j.gexplo.2018.03.008 Received 14 May 2017; Received in revised form 12 March 2018; Accepted 14 March 2018 Available online 16 March 2018 0375-6742/ © 2018 Elsevier B.V. All rights reserved. important geochemical processes dominating arsenic mobilization during short-term artificial flooding.

Arsenic behavior can be well modeled using reactive transport modeling, which is commonly applied to simulate or reconstruct geochemical processes in groundwater along a flow path, based on the advection-dispersion-reaction equations (Parkhurst and Appelo, 1999b). Charlet et al. (2007) coupled field monitoring and reactive transport modeling to study the controlling geochemical processes of arsenic cycling in Chakdaha, India, identifying the important role of  $PO_4^{3-}$ ,  $HCO_3^{-}$  and Fe(II) in mobilizing the arsenic plume. In the same setting, Burnol and Charlet (2010) developed a 1D reactive transport model of growing complexity to simulate the transition between a less reduced and more reduced environment, for comparison with field data. Their results showed that microbial sulfate reduction followed by abiotic and/or biotic reduction of As(III)-bearing iron oxides accounted for the spatial heterogeneity of arsenic in such reduced aquifers. In order to elucidate the fate of arsenic and its co-contaminants that prevail in a coastal aquifer subject to salt-water intrusion, Colombani et al. (2015) constructed a two-dimensional reactive transport model based on data obtained at an arsenic contaminated site bordering the Mediterranean Sea. The modeling suggested that in the sub-oxic zone an influx of oxygenated water promoted arsenic attenuation via coprecipitation with arsenic and iron oxides and copper hydroxides. In contrast, in the deeper aquifer zone, iron reduction associated with the release of adsorbed arsenic and dissolution of arsenic bearing phases, provided a persistent source for groundwater pollution. Postma et al. (2016) used 1D reactive transport modeling to comprehensively quantify the effect of early diagenesis of Holocene sediments in an arsenic contaminated aquifer, and elucidate how early diagenesis affected the groundwater arsenic content.

Until now, however, reactive transport modeling has rarely been applied to illustrate the mechanism of arsenic enrichment in groundwater during surface water-groundwater interactions. Here we present a first attempted to quantify the arsenic mobilization in the shallow groundwater system of the Datong Basin during a period of extensive surface water-groundwater interaction. Towards this objective we have used and extended the datasets obtained from an experimental field site (Fig. 1) in Datong Basin (Yu et al., 2015; Xie et al., 2015). At this site, short-term artificial flooding has been conducted and the water chemistry and arsenic concentration variations have been monitored during these controlled hydrologic events. Here we use these data to analyze the geochemical processes and changes occurring with flooding. We, incorporate the data into a model, which adds elements of growing complexity, including surface complexation model and 1D reactive transport, to quantify and predict how groundwater chemistry, including arsenic concentrations, changes during surface-groundwater interactions. Our results help to understand the main geochemical processes controlling arsenic mobilization in the shallow groundwater system and provide new insight into arsenic behavior in groundwater during transient hydrological events such as short-term floods.

#### 2. Study site

The 75-m long and 30-m wide Shanyin Field Site (SYFS) is adjacent to the Sanggan River in Shanyin country of the central Datong Basin (Fig. 1a). A series of boreholes was drilled and multi-level piezometer nests installed along a transect perpendicular to the river channel. Three Quaternary sand aquifers were encountered (sand 1, sand 2, and sand 3), with a thickness of approximately 1.5 m, 3 m, and 4 m respectively, separated by three thin clay aquitards (clay 1, clay 2, and clay 3) with thicknesses of approximately 1 m, 3 m, and 2 m respectively (Fig. 1c). The 0–10 m deep sediments overlying clay 1 are composed of unconsolidated silt and discontinuously occurring clay lenses. The riverbed sediments consist of sand, sandy silt and silt. According to the results of relative elevation of the drill site (not shown) and a previous hydrogeological survey (Shanxi Geological Survey, 1981), the topography is very flat.

As the major surface water system in this basin, the Sanggan River is an ephemeral river which has ceased flow for many years, apart from during artificial flooding in October each year from the Dongyulin reservoir that is 20 km upstream of the site (Fig. 1a), functioning as the source for seasonal irrigation at Datong. Further details of the artificial flooding experiment on which this study is based were presented in Yu et al. (2015).

#### 2.1. Water chemistry evolution during the flood

According to Yu et al. (2015), there was extensive mixing of surface water and groundwater during the flood, illustrated by the following lines of evidence: 1) groundwater levels, especially those in the shallow aquifer, fluctuated in agreement with surface water levels. The surface water level fluctuated with time in a range of over 80 cm. The groundwater level increased by almost 30 cm in wells located 5 m away from the river and over 15 cm in wells located 80 m away from the river; 2) an increase in  $\delta^{18}$ O and  $\delta^{2}$ H values of shallow groundwater samples occurred; 3) a shift in <sup>87</sup>Sr/<sup>86</sup>Sr ratios of post-flood groundwater samples towards those of surface water occurred; 4) increases in  $Mg^{2+}$ ,  $Na^{+}$ ,  $Ca^{2+}$  and  $SO_4^{2-}$  concentration occurred simultaneously in groundwater and surface water. This study also documented that significant increases in arsenic concentrations after the flood occurred, likely related to the oxidation of organic matter, reductive dissolution of Fe-oxyhydroxides and bacterially-mediated reactions. Aside from these factors, arsenic desorption from iron oxide surfaces at high pH, and competitive sorption with bicarbonate may also have elevated arsenic concentrations as demonstrated in many other oxic systems (Currell et al., 2011). The data in Yu et al. (2015) provided insight into the possible processes controlling arsenic mobilization in the groundwater system during the flood, however, which of these processes was dominant, or which were of greater or lesser importance were not clarified. To address this remaining uncertainty, a 1D reactive transport model coupled arsenic (bio)geochemical processes was constructed to clarify the dominant processes controlling arsenic mobilization in the groundwater system during the short-term artificial flood.

#### 3. Methods

The "1D reactive transport model" was constructed based on the data reported in the previous study of Yu et al. (2015), which indicated that only shallow groundwater chemistry conspicuously fluctuated in response to the flood. Consequently, the model focused on the shallow groundwater system, scilicet 1-10 m in the X direction and -10 to -11 m in the Z direction (X indicates the horizontal distance from the river; Z indicates the vertical distance from the ground surface) (Fig. 2). Only the monitoring wells 1-2S and 2-2S were included in this model. The main purpose of the model was to simulate the advection-dispersion-reaction processes in a 1D horizontal column with continuous flow. In order to test alternative hypotheses and better understand the mechanism of arsenic mobilization in groundwater during the flood, two models were tested: iron(III) surface complexation model and 1D generic reactive transport model. Practically, two sub-models were involved in the 1D generic reactive transport model. Sub-model (a) only included the redox reaction processes, i.e. the reduction dissolution of SO<sub>4</sub><sup>2-</sup>, NO<sub>3</sub><sup>-</sup>, As(V) and solid Fe(III) and FeS<sub>2</sub>; sub-model (b) included both the surface complexation reactions on Fe(III) and the above redox reaction processes. By comparing the calibration results of the three models, we could figure out the dominant processes controlling arsenic mobilization in Datong groundwater during surface water and groundwater interactions. Details of each model are provided in the following sections.

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