Hydrological cycle, hydrogeological characteristics and mobility of arsenic in groundwater in watershed of Nanfei river, Anhui, China

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Arsenic (As), which is ubiquitous in the environment, has been recognized as one of the most widespread and problematic water contaminants. This study has investigated the hydrological cycle, hydrochemical characteristics and the As contamination of groundwater in the Nanfei watershed between Chaohu lake and old town of Hefei, China. An attempt was made to study the relationship among the hydrological cycle, hydrogeological characteristics and mobility of As in groundwater at Nanfei river watershed. Groundwater samples were collected at 45 locations in the area of Nanfei river watershed. The relationships among the three factors are analyzed. Results show that: (1) There were very variable chemical composition of groundwater. 44% groundwater was of Na-HCO_3 type, and 40% groundwater was of Ca-HCO_3 type. Most groundwater was alkalescence and the groundwater chemistry was more influenced by landuse and town development; (2) The hydrological cycle of a aquifer plays important roles in the release of As to groundwater. The observed groundwater flow lines of the aquifer indicates that groundwater movement is very slow in the As-contaminated area. In addition, there are higher As concentration in the area where the aquifers are recharged by the drainage from city. (3) The high As concentration occur in anaerobic groundwaters from the study area associated with moderately high dissolved Fe as well as high Mn, NH_4^+, and SO_4^{2-} concentration, through the investigation of Nanfei river watershed, Anhui, China. The results will provide scientific insights from a broad hydrogeochemical perspective that will guide sustainable management of contaminant-safe aquifers for Hefei city.

This study was supported by the National Natural Science Foundation of China (No.40672154 and No.40772153), Program for New Century Excellent Talents in University (No. NCET-06-0541)

Mapping the iron-binding site on the small tetraheme cytochrome of *Shewanella oneidensis* MR-1

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Shewanella oneidensis MR-1 has the metabolic capacity to grow anaerobically under Fe(III)-reducing condition in which it produces a variety of periplasmic *c*-type cytochromes that are thought to be involved in the Fe(III) respiratory process. Among those is the small tetraheme cytochrome (SoSTC) with unknown physiological role although its homologous form from *Shewanalla frigidimarina* has been proved to participate in iron respiration. In this work, biochemical studies were conducted to characterize the iron binding affinities and to identify the iron-binding site on SoSTC. We use Isothermal Titration Calorimetry (ITC) to measure binding affinities between purified recombinant SoSTC and various Fe (III)-chelates including Fe (III)-EDTA*, Fe (III)-NTA*, and Fe (III)-Citrate. The ITC measurements demonstrate that SoSTC has a preferential binding with Fe (III)-EDTA and Fe(III)-NTA with dissociation constant (K_d) around 2 mM over Fe(III)-Citrate with K_d larger than 1 mM. The iron binding constants have also been quantitated by iron-dependent transient kinetics using stopped flow. Both ITC measurements and transient kinetics have shown comparable binding affinity values. Interestingly, there is little binding between SoSTC with NTA alone suggesting that the binding event occurred between SoSTC and Fe(III)-NTA complex. In contrast with ferric species, ferrous chelates have shown about 10-100 times less in terms of binding affinity with SoSTC.

With understanding of SoSTC binding with charged iron complex, we propose that the iron binding site should consist of charged amino acids. Through chemical modification of amine groups and carboxyl groups, we have found that SoStc with carboxyl residues modified to amine groups shows no binding with Fe(III)-EDTA by ITC measurements. Moreover, the electron transfer rate constant of carboxyl-group modified SoSTC when reacting with Fe (III)-EDTA were retarded by 50 times. Carboxyl-group scanning studies were used to probe the putative iron-binding site by site-directed mutagenesis of glutamate and aspartate on SoStc. ITC and Stopped flow were then used to characterize the binding between SoStc purified from each mutant with Fe (III)-EDTA. SoStc (D79N) shows no binding with Fe(III)-EDTA measured from calorimetric measurements. The imparity of the binding of SoSTC (D79N) with Fe (III)-EDTA was further confirmed by transient state kinetics of reduced SoSTC (D79N) reacting with Fe (III)-EDTA which demonstrates around 10 times decrease of second order rate constant. Thus, we suggest that Asp^{79} is involved in iron binding on SoSTC.