Imaging geochemical heterogeneities using inverse reactive transport modeling: An example relevant for characterizing arsenic mobilization and distribution

The spatial distribution of reactive minerals in the subsurface is often a primary factor controlling the fate and transport of contaminants in groundwater systems. However, direct measurement and estimation of heterogeneously distributed minerals are often costly and difficult to obtain. While previous studies have shown the utility of using hydrologic measurements combined with inverse modeling techniques for tomography of physical properties including hydraulic conductivity, these methods have seldom been used to image reactive geochemical heterogeneities. In this study, we focus on As-bearing reactive minerals as aquifer contaminants. We use synthetic applications to demonstrate the ability of inverse modeling techniques combined with mechanistic reactive transport models to image reactive mineral lenses in the subsurface and quantify estimation error using indirect, commonly measured groundwater parameters. Specifically, we simulate the mobilization of arsenic via kinetic oxidative dissolution of As-bearing pyrite due to dissolved oxygen in the ambient groundwater, which is an important mechanism for arsenic release in groundwater both under natural conditions and engineering applications such as managed aquifer recharge and recovery operations. The modeling investigation is carried out at various scales and considers different flow-through domains including (i) a 1D lab-scale column (SO cm), (ii) a 2D lab-scale setup (60 cm x 30 cm) and (iii) a 2D field scale domain (20 m x 4 m). In these setups, synthetic dissolved oxygen data and forward reactive transport simulations are used to image the spatial distribution of As-bearing pyrite using the Principal Component Geostatistical Approach (PCGA) for inverse modeling. (C) 2015 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Environmental Engineering, Water Resources Engineering, Stanford University
Contributors: Fakhreddine, S., Lee, J., Kitanidis, P. K., Fendorf, S., Rolle, M.
Number of pages: 12
Pages: 186-197
Publication date: 2016
Peer-reviewed: Yes

Publication information
Journal: Advances in Water Resources
Volume: 88
ISSN (Print): 0309-1708
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.49 SJR 1.551 SNIP 1.561
Web of Science (2017): Impact factor 3.512
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.53 SJR 2.202 SNIP 2.036
Web of Science (2016): Impact factor 3.221
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.31 SJR 2.24 SNIP 2.062
Web of Science (2015): Impact factor 4.349
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.66 SJR 1.951 SNIP 1.951
Web of Science (2014): Impact factor 3.417
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.03 SJR 1.432 SNIP 1.748
Web of Science (2013): Impact factor 2.78
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1